Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 11:09 am BST

PDB ID	:	7O1C
EMDB ID	:	EMD-12695
Title	:	Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome-RF2 complex stalled in response to L-tryptophan
Authors	:	van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on	:	2021-03-29
Resolution	:	2.60 Å(reported)
Based on initial model	:	6TBV

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

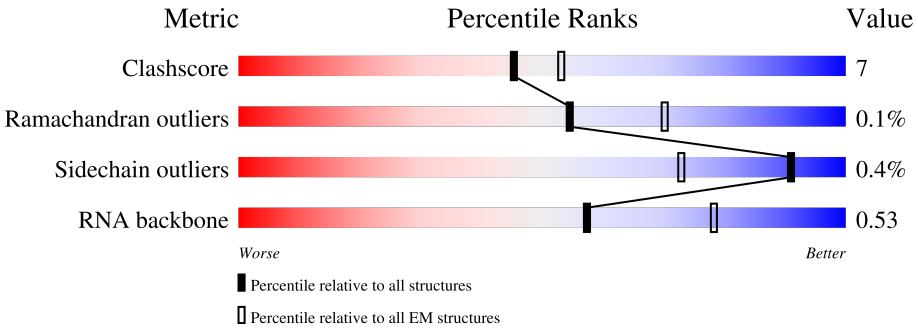
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	50% 33% 15%
2	AB	241	23% 71% 20% 7%
3	AC	233	62% 26% 12%
4	AD	206	81% 18%
5	AE	167	74% 19% 7%
6	AF	135	56% 20% 21%
7	AG	179	61% 23% 16%

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Mol	Chain	Length	Quality of chain
8	AH	130	75% 23%
9	AI	130	9% 62% 35%
10	AJ	103	30% 59% 35%
11	AK	129	64% 27% 9%
12	AL	124	75% 23%
13	AM	118	69% 28%
14	AN	102	70% 28%
15	AO	89	96%
16	AP	82	80% 20%
17	AQ	84	74% 21% 5%
18	AR	75	55% 19% 27%
19	AS	92	5% 57% 30% 11%
20	AT	87	87% 11%
21	AU	71	56% 21% 21%
22	BA	2897	48% 37% 13%
23	BB	120	61% 28% 10%
24	BC	273	80% 18%
25	BD	209	82% 17%
26	BE	201	5% 84% 16%
27	BF	179	72% 27%
28	BG	177	82% 16%
29	BH	149	51% 65% 35%
30	BI	70	34% 53% 40% 6%
31	BJ	142	84% 15%
32	BK	123	87% 13%

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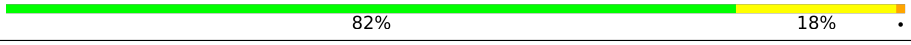
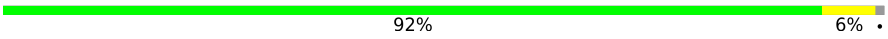
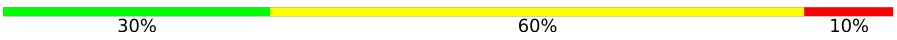
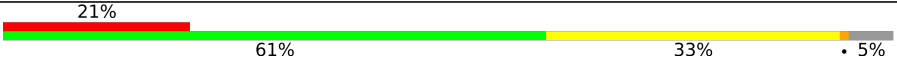
Mol	Chain	Length	Quality of chain
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	B5	17	
54	B7	10	
55	B8	77	
56	B9	365	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148175 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1534	32930	14694	6041	10661	1534	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	155	1144	711	216	211	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	BQ	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	BU	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	B1	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called TnaC-(R23F) - Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	10	Total	C	N	O	P	0	0
			211	94	36	71	10		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 56 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B9	348	Total	C	N	O	S	0	0
			2768	1705	482	571	10		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	87	Total	Mg	0
			87	87	
57	BA	243	Total	Mg	0
			243	243	
57	BB	1	Total	Mg	0
			1	1	
57	BC	1	Total	Mg	0
			1	1	
57	BD	2	Total	Mg	0
			2	2	
57	BL	3	Total	Mg	0
			3	3	
57	B8	2	Total	Mg	0
			2	2	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	AA	38	Total	K	0
			38	38	
58	AM	1	Total	K	0
			1	1	
58	BA	104	Total	K	0
			104	104	
58	BB	1	Total	K	0
			1	1	
58	BC	1	Total	K	0
			1	1	
58	BD	1	Total	K	0
			1	1	

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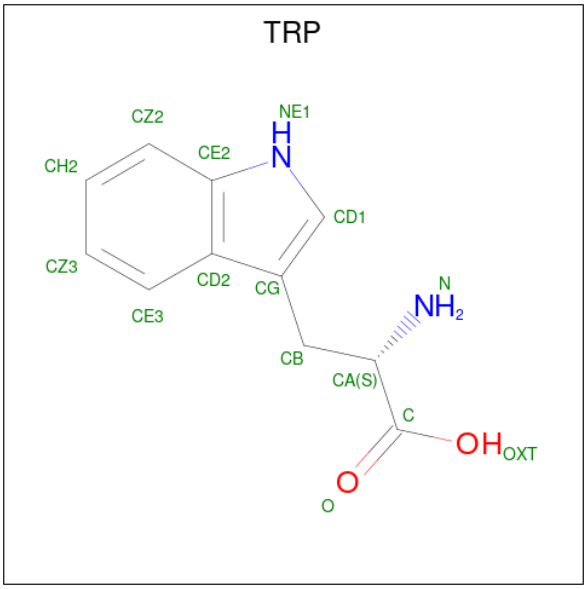
Mol	Chain	Residues	Atoms	AltConf
58	BM	1	Total K 1 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	AB	1	Total Zn 1 1	0
59	BI	1	Total Zn 1 1	0
59	B4	1	Total Zn 1 1	0

- Molecule 60 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms	AltConf
60	BA	1	Total C N O 15 11 2 2	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	AA	167	Total O 167 167	0
61	AK	1	Total O 1 1	0

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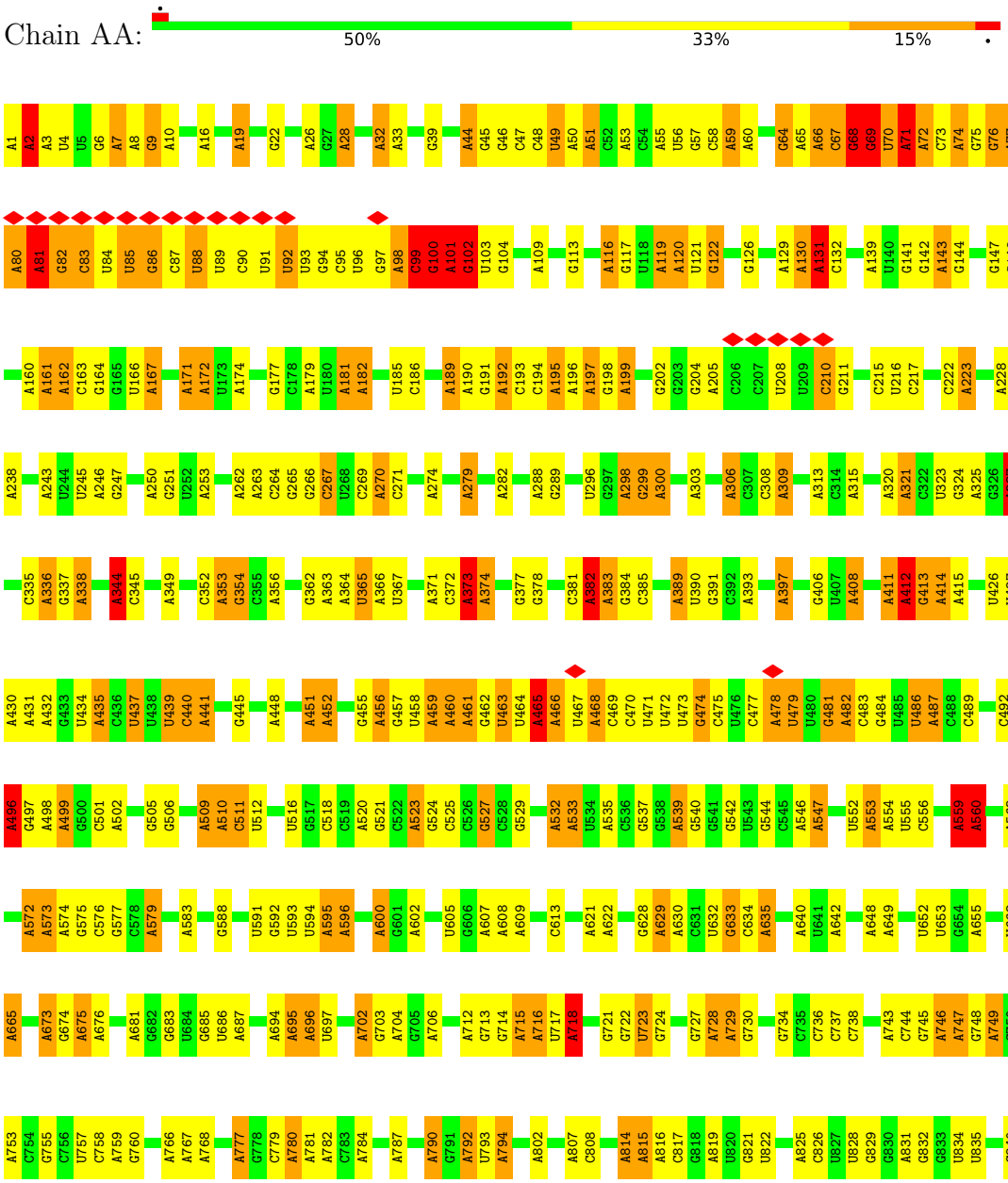
Mol	Chain	Residues	Atoms	AltConf
61	AM	1	Total O 1 1	0
61	AN	3	Total O 3 3	0
61	BA	617	Total O 617 617	0
61	BC	6	Total O 6 6	0
61	BD	2	Total O 2 2	0
61	BN	3	Total O 3 3	0

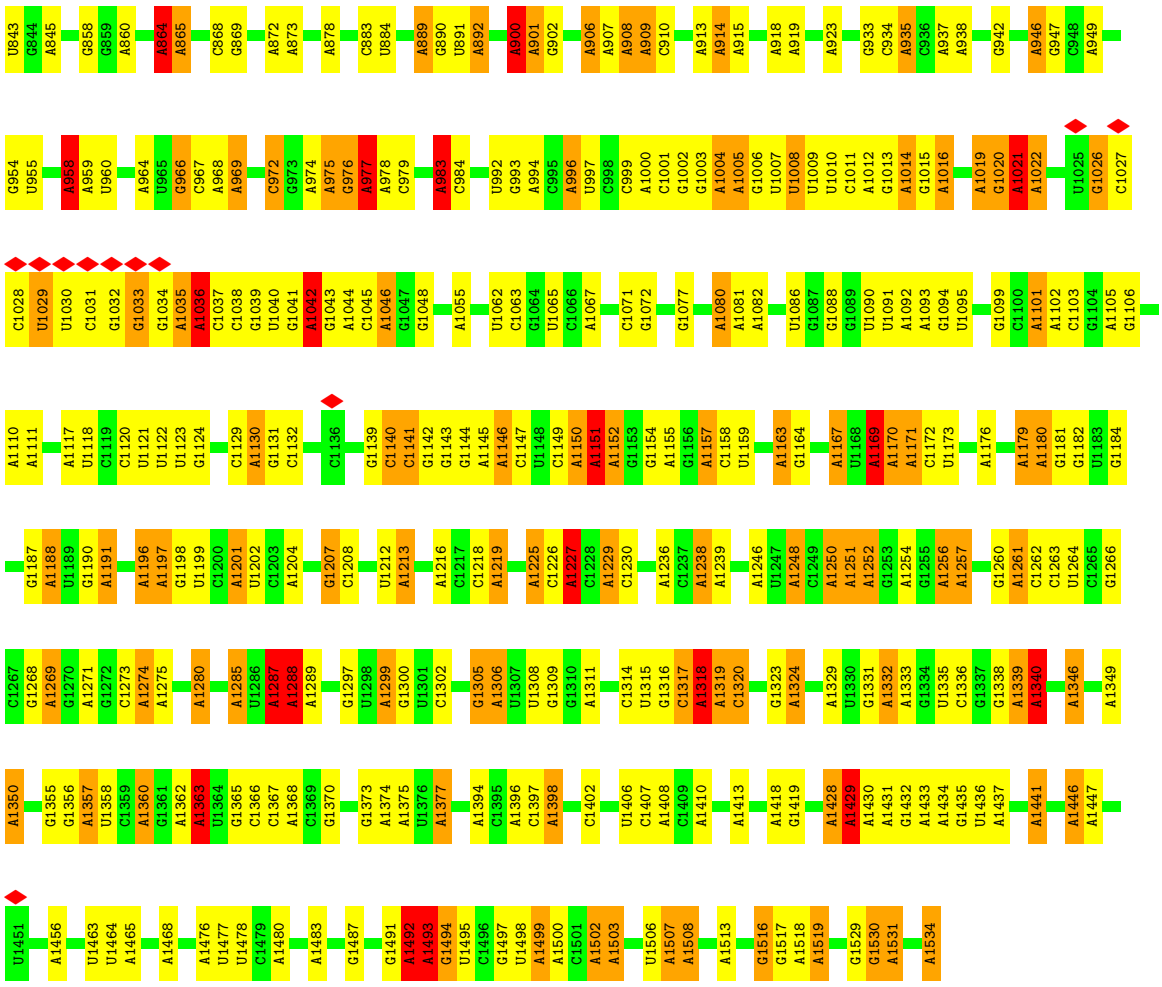
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribosomal RNA 16S

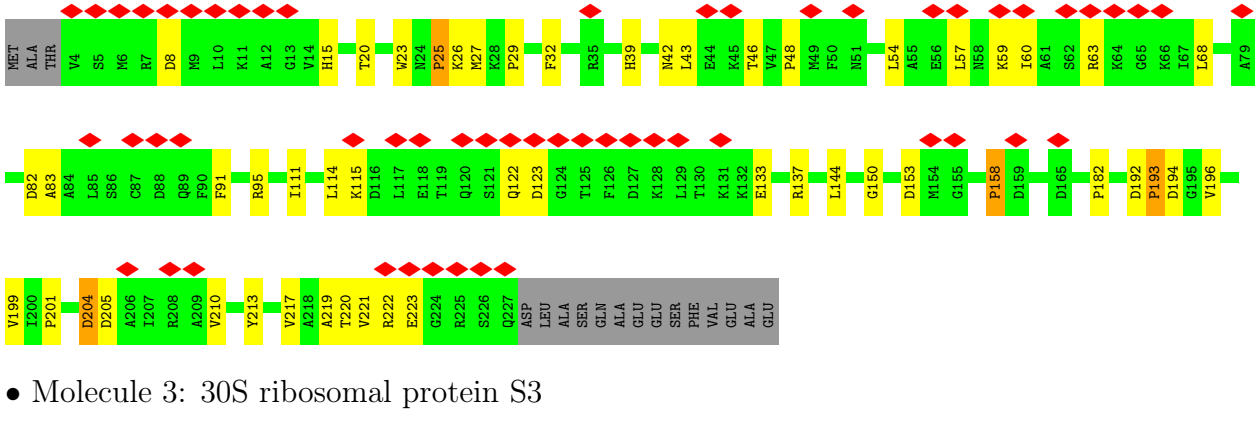
Chain AA:





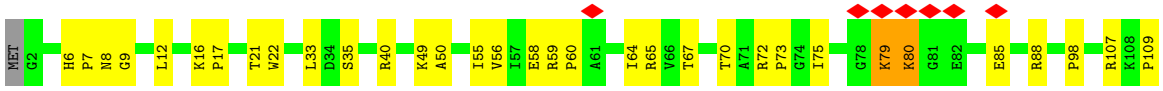
• Molecule 2: 30S ribosomal protein S2

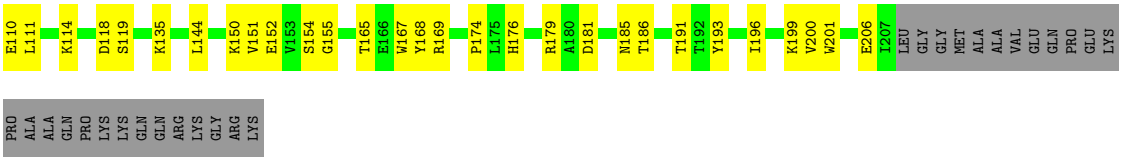
Chain AB:



• Molecule 3: 30S ribosomal protein S3

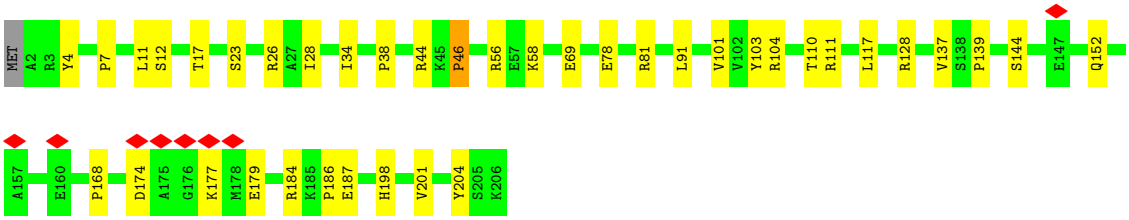
Chain AC:





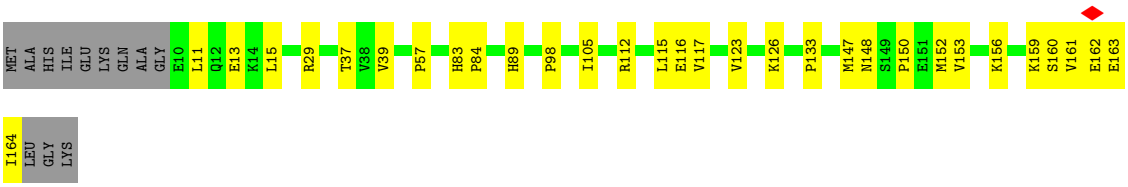
• Molecule 4: 30S ribosomal protein S4

Chain AD:



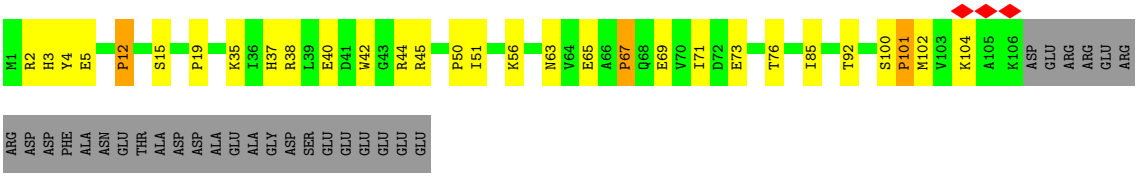
• Molecule 5: 30S ribosomal protein S5

Chain AE:



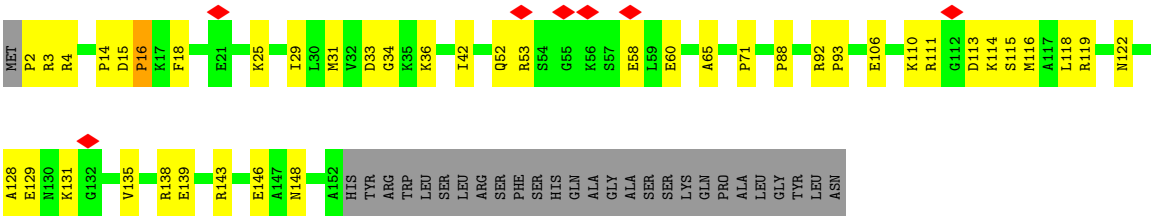
• Molecule 6: 30S ribosomal protein S6

Chain AF:



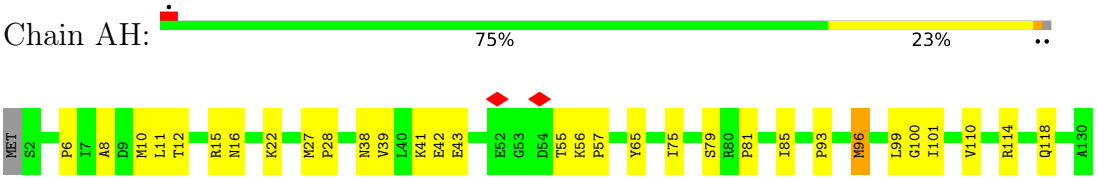
• Molecule 7: 30S ribosomal protein S7

Chain AG:



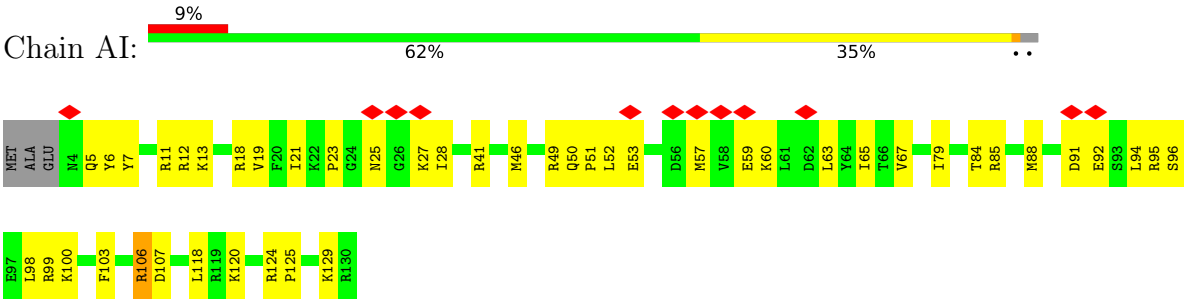
• Molecule 8: 30S ribosomal protein S8

Chain AH:



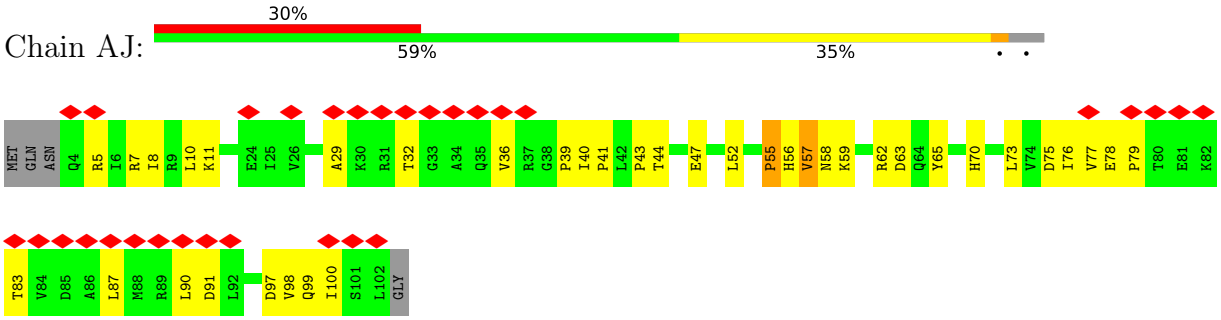
• Molecule 9: 30S ribosomal protein S9

Chain AI:



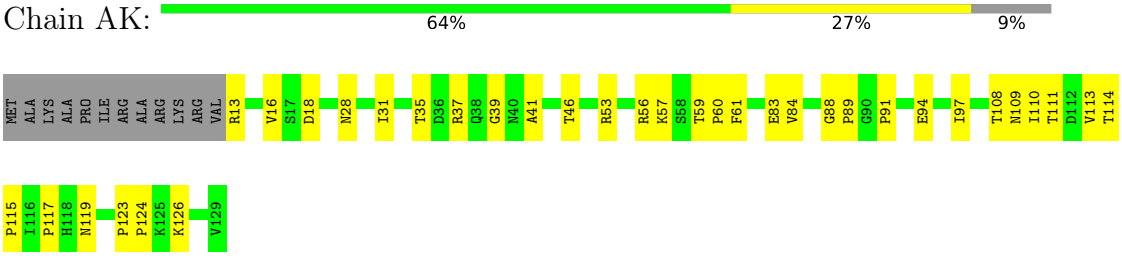
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



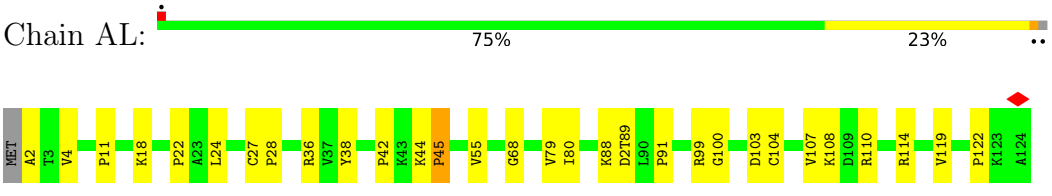
• Molecule 11: 30S ribosomal protein S11

Chain AK:



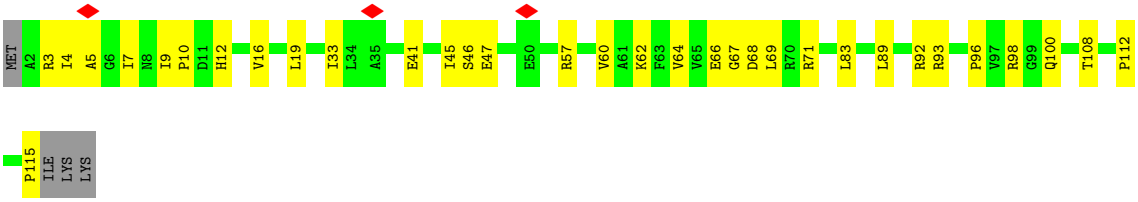
• Molecule 12: 30S ribosomal protein S12

Chain AL:

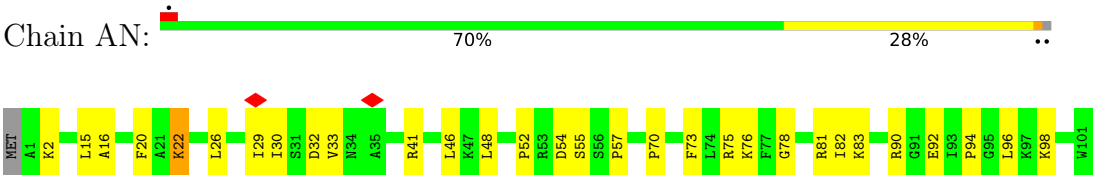


• Molecule 13: 30S ribosomal protein S13

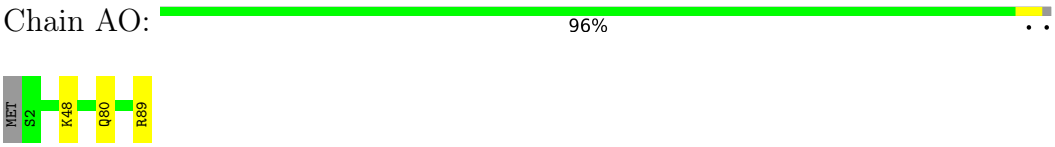
Chain AM:



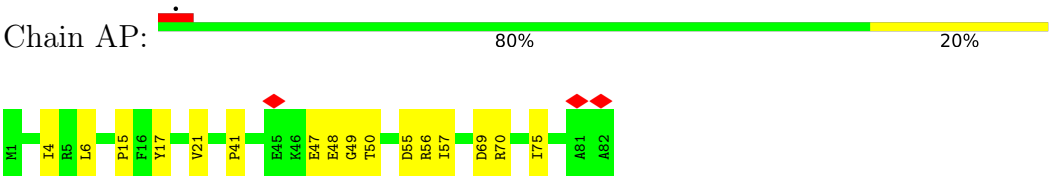
• Molecule 14: 30S ribosomal protein S14



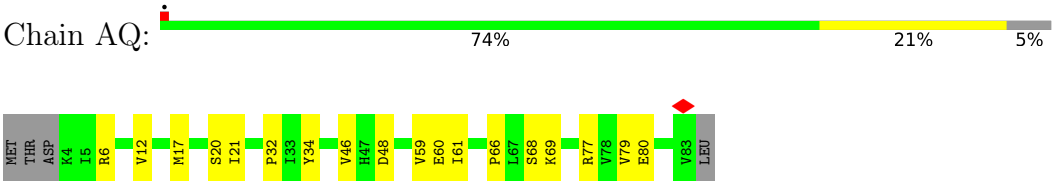
• Molecule 15: 30S ribosomal protein S15



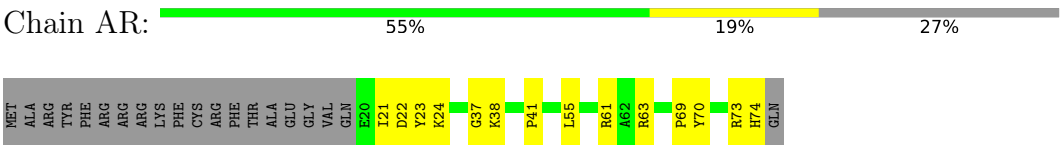
• Molecule 16: 30S ribosomal protein S16



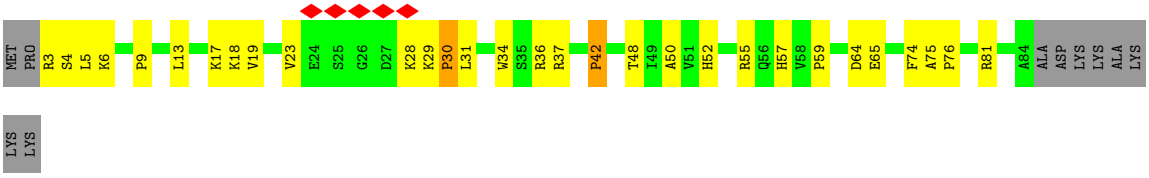
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

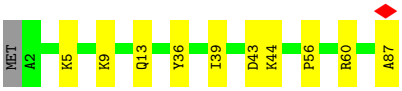


• Molecule 19: 30S ribosomal protein S19



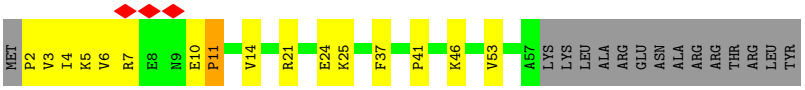
• Molecule 20: 30S ribosomal protein S20

Chain AT:



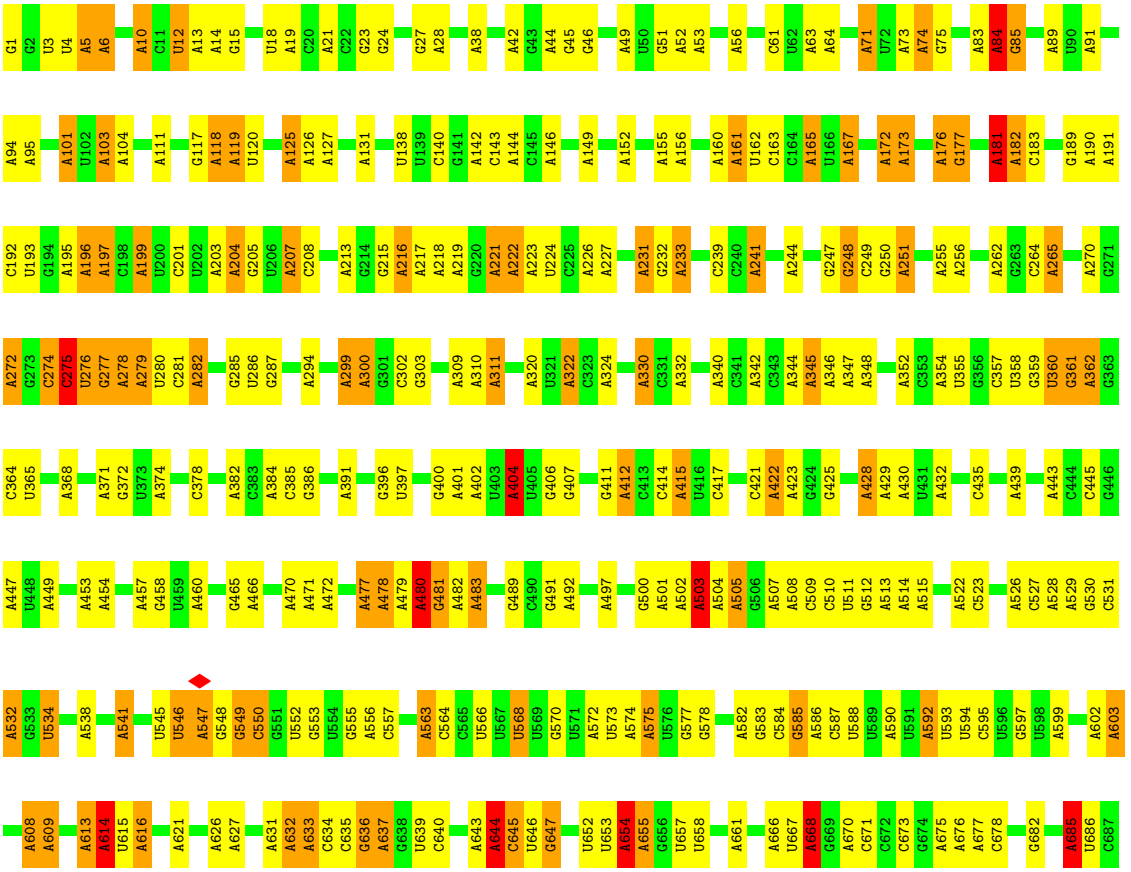
• Molecule 21: 30S ribosomal protein S21

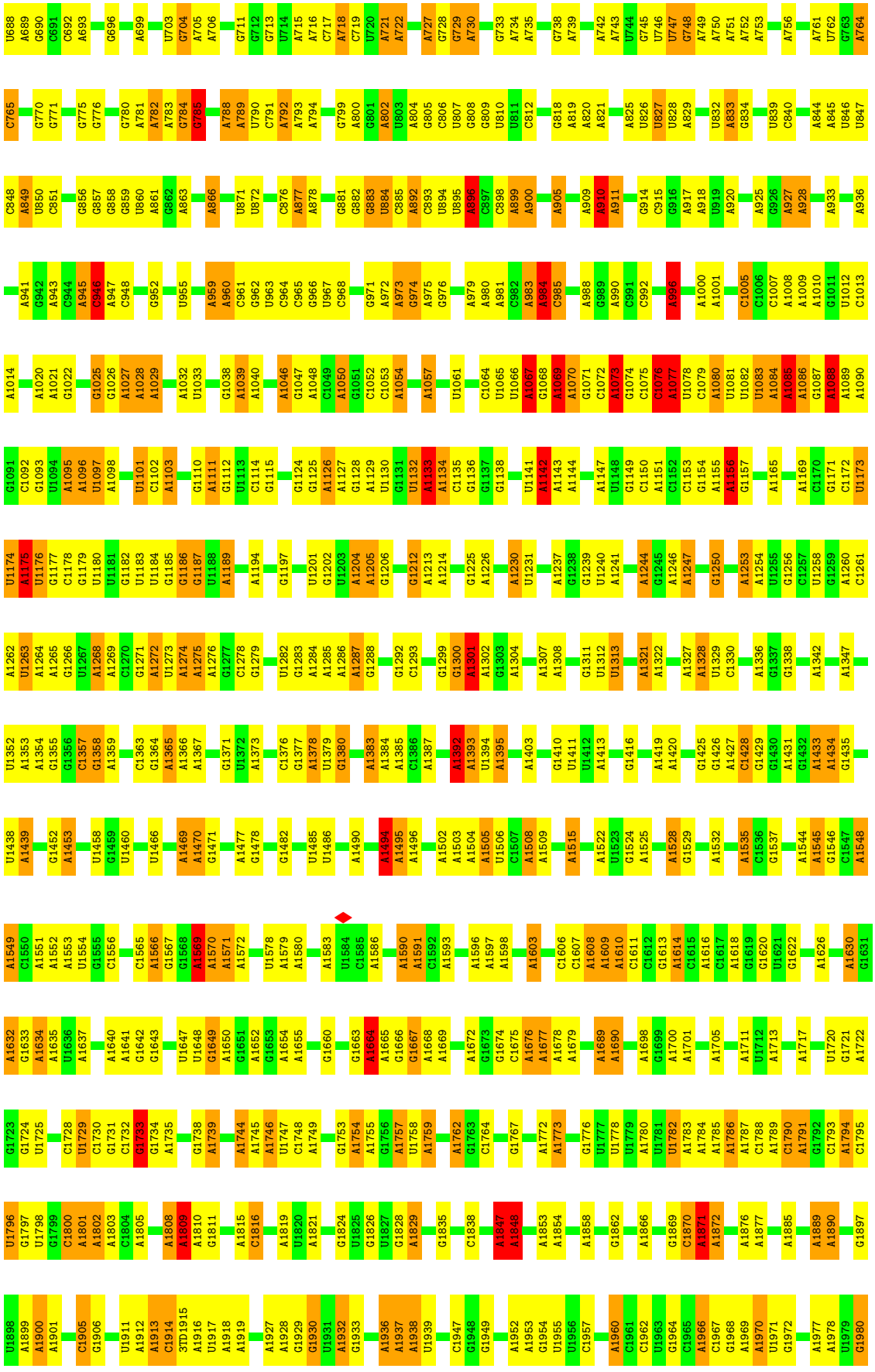
Chain AU:

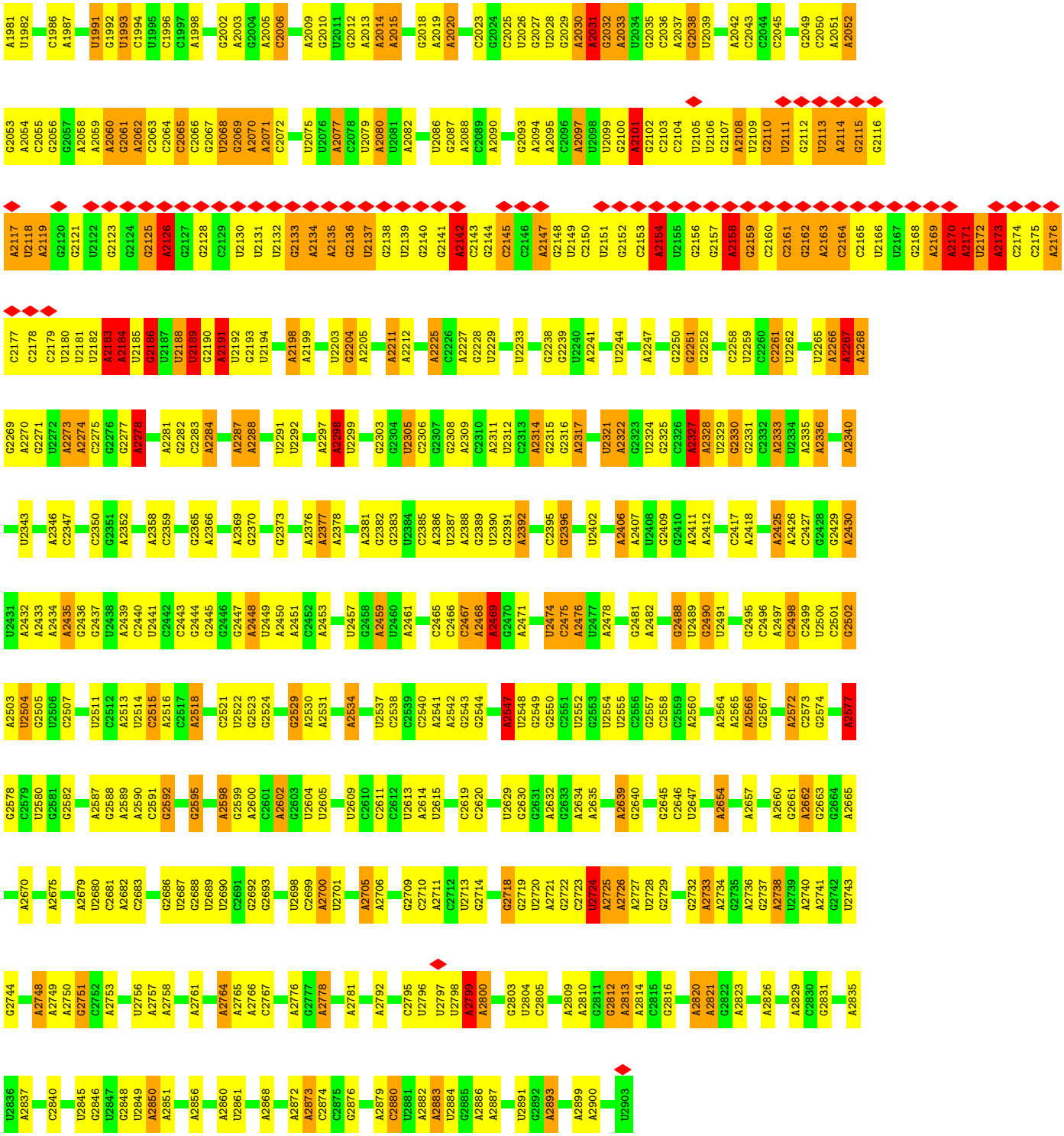


• Molecule 22: Ribosomal RNA 23S

Chain BA:





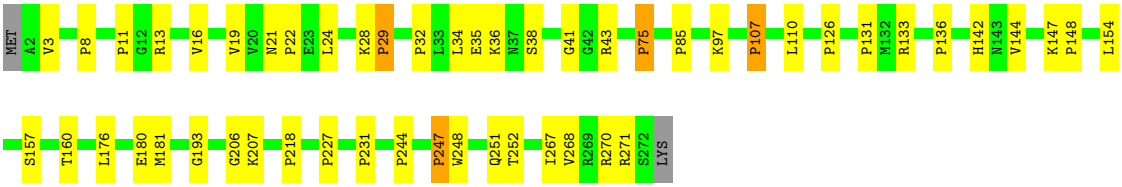


• Molecule 23: Ribosomal RNA 5S

Chain BB:

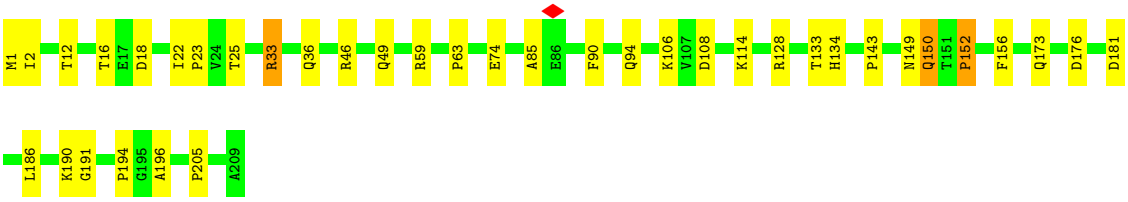
• Molecule 24: 50S ribosomal protein L2

Chain BC:



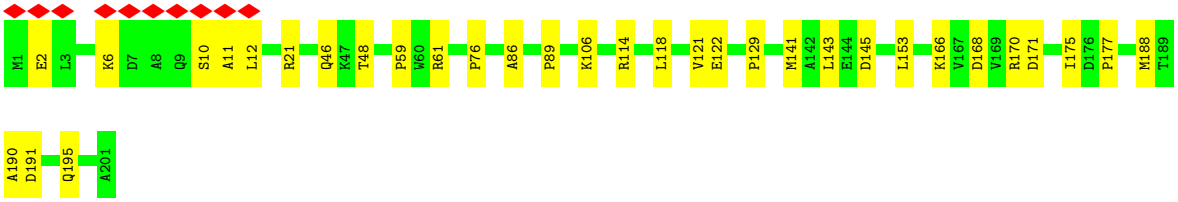
• Molecule 25: 50S ribosomal protein L3

Chain BD:



• Molecule 26: 50S ribosomal protein L4

Chain BE:

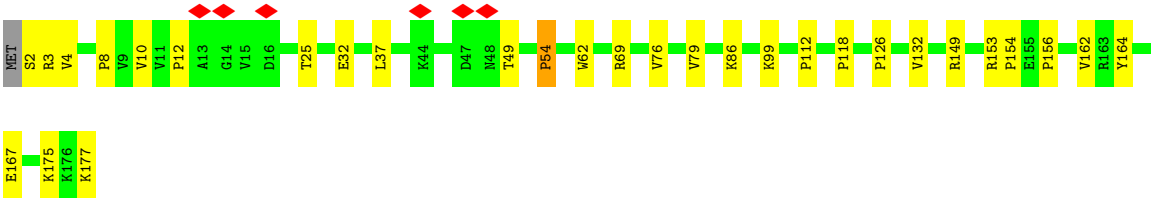


• Molecule 27: 50S ribosomal protein L5

Chain BF:

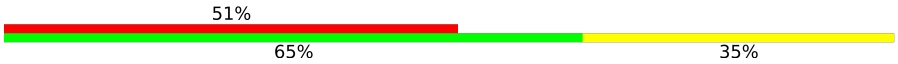
• Molecule 28: 50S ribosomal protein L6

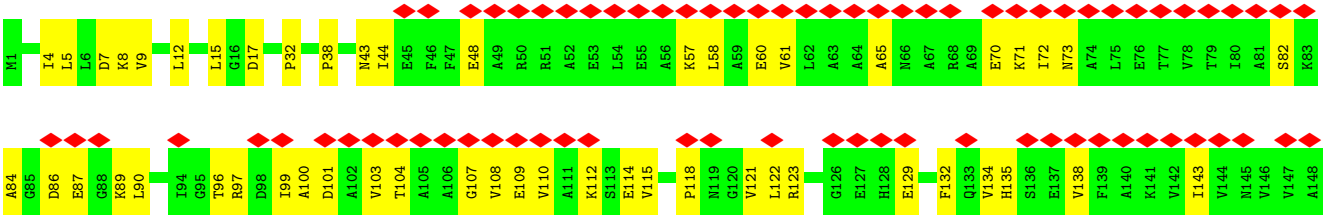
Chain BG:



• Molecule 29: 50S ribosomal protein L9

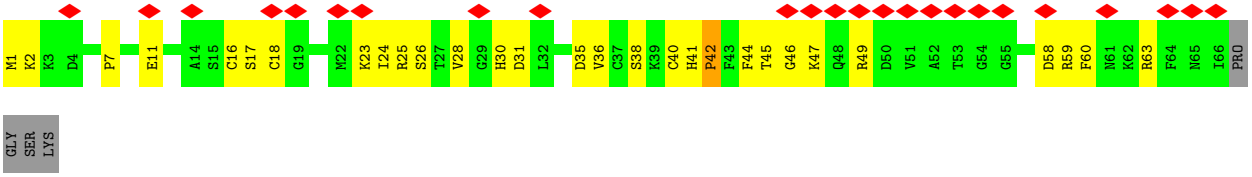
Chain BH:





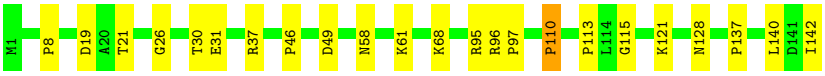
• Molecule 30: 50S ribosomal protein L31

Chain BI:



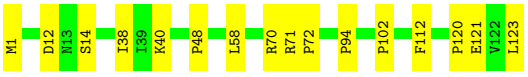
• Molecule 31: 50S ribosomal protein L13

Chain BJ:



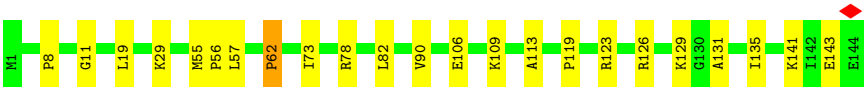
• Molecule 32: 50S ribosomal protein L14

Chain BK:



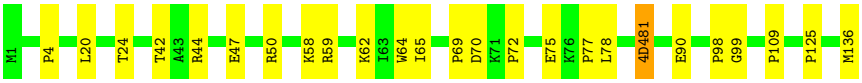
• Molecule 33: 50S ribosomal protein L15

Chain BL:



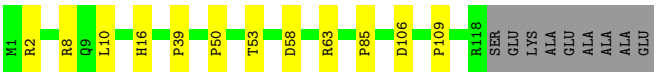
• Molecule 34: 50S ribosomal protein L16

Chain BM:



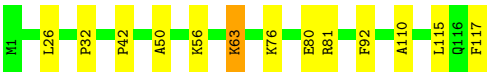
• Molecule 35: 50S ribosomal protein L17

Chain BN:



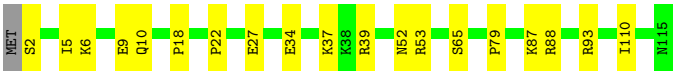
• Molecule 36: 50S ribosomal protein L18

Chain BO:



• Molecule 37: 50S ribosomal protein L19

Chain BP:

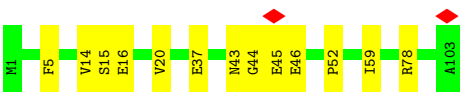


• Molecule 38: 50S ribosomal protein L20

Chain BQ:

• Molecule 39: 50S ribosomal protein L21

Chain BR:

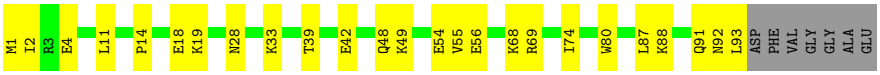


• Molecule 40: 50S ribosomal protein L22

Chain BS:

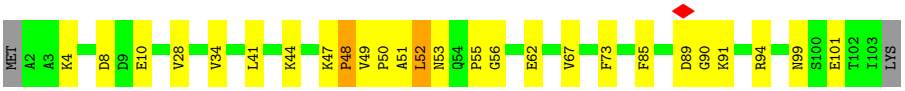
• Molecule 41: 50S ribosomal protein L23

Chain BT:



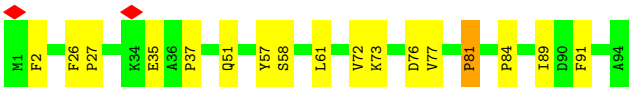
• Molecule 42: 50S ribosomal protein L24

Chain BU:



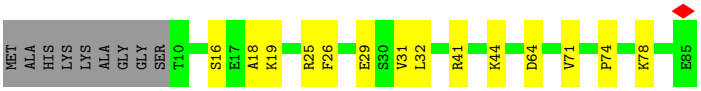
• Molecule 43: 50S ribosomal protein L25

Chain BV:



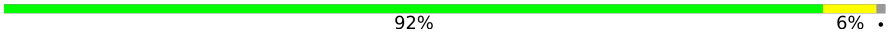
• Molecule 44: 50S ribosomal protein L27

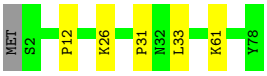
Chain BW:



• Molecule 45: 50S ribosomal protein L28

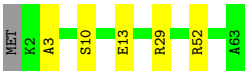
Chain BX:





• Molecule 46: 50S ribosomal protein L29

Chain BY:

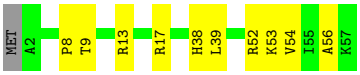


• Molecule 47: 50S ribosomal protein L30

Chain BZ:

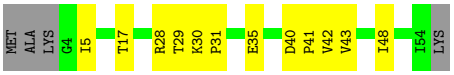
• Molecule 48: 50S ribosomal protein L32

Chain B0:



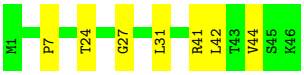
• Molecule 49: 50S ribosomal protein L33

Chain B1:



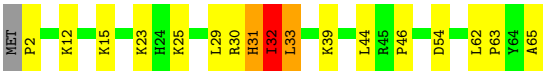
• Molecule 50: 50S ribosomal protein L34

Chain B2:



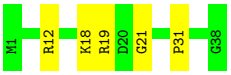
• Molecule 51: 50S ribosomal protein L35

Chain B3:



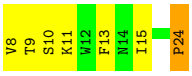
• Molecule 52: 50S ribosomal protein L36

Chain B4:



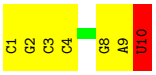
• Molecule 53: TnaC-(R23F) - Tryptophanase leader peptide

Chain B5:



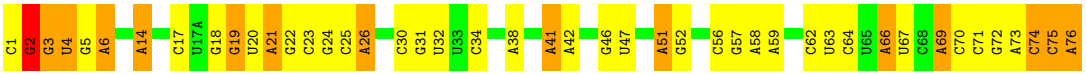
• Molecule 54: mRNA

Chain B7:



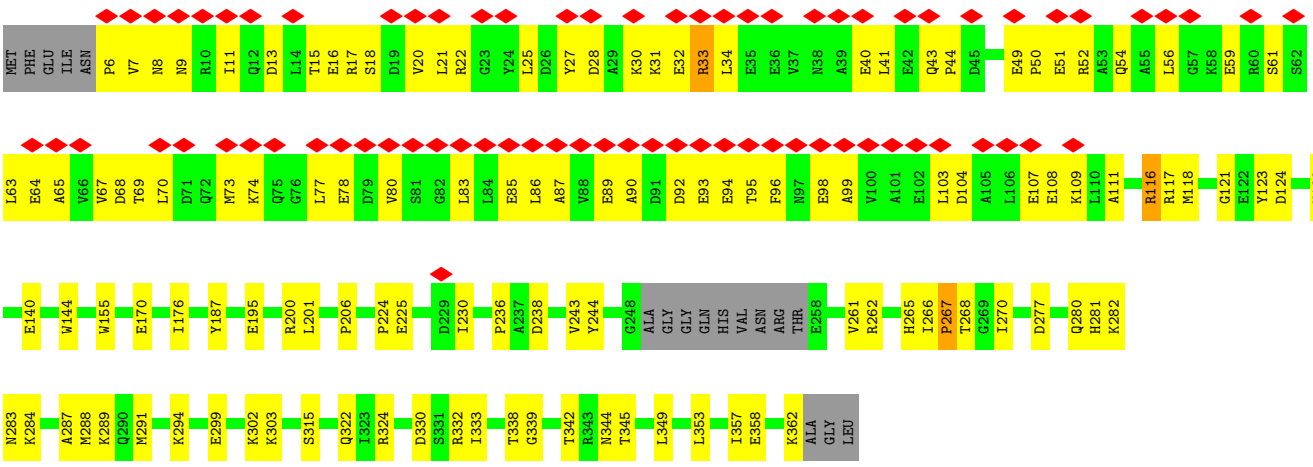
• Molecule 55: P-site tRNA-Pro

Chain B8:



• Molecule 56: Peptide chain release factor RF2

Chain B9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose ($e^-/Å^2$)	40, 44	Depositor
Minimum defocus (nm)	-1000, -400	Depositor
Maximum defocus (nm)	-2000, -1600	Depositor
Magnification	55127, 59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	370.056, 370.056, 370.056	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.907, 0.907, 0.907	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 5MU, K, 6MZ, 3TD, D2T, MEQ, 2MG, MA6, 4OC, 2MA, 5MC, MG, 1MG, OMC, OMG, ZN, OMU, PSU, 4D4, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	1.65	964/36593 (2.6%)	3.44	4347/57081 (7.6%)
2	AB	0.82	7/1784 (0.4%)	0.56	1/2403 (0.0%)
3	AC	0.86	7/1651 (0.4%)	0.62	2/2225 (0.1%)
4	AD	0.81	6/1665 (0.4%)	0.51	0/2227
5	AE	0.90	5/1157 (0.4%)	0.60	0/1557
6	AF	1.01	5/881 (0.6%)	0.56	0/1189
7	AG	0.96	7/1195 (0.6%)	0.54	0/1602
8	AH	0.94	5/989 (0.5%)	0.62	1/1326 (0.1%)
9	AI	0.76	3/1034 (0.3%)	0.56	0/1375
10	AJ	1.05	6/805 (0.7%)	0.59	0/1089
11	AK	1.11	7/893 (0.8%)	0.62	0/1205
12	AL	1.18	8/960 (0.8%)	0.65	0/1286
13	AM	0.93	5/892 (0.6%)	0.58	0/1193
14	AN	0.89	4/811 (0.5%)	0.55	0/1081
15	AO	0.44	0/722	0.48	0/964
16	AP	0.76	2/659 (0.3%)	0.60	0/884
17	AQ	0.83	2/657 (0.3%)	0.55	0/881
18	AR	0.97	2/462 (0.4%)	0.58	0/621
19	AS	1.09	5/672 (0.7%)	0.65	0/904
20	AT	0.60	1/676 (0.1%)	0.46	0/895
21	AU	1.09	4/472 (0.8%)	0.53	0/627
22	BA	2.12	2046/69120 (3.0%)	3.57	8225/107824 (7.6%)
23	BB	1.74	59/2872 (2.1%)	3.03	258/4478 (5.8%)
24	BC	1.29	23/2121 (1.1%)	0.68	0/2852
25	BD	1.05	11/1576 (0.7%)	0.64	0/2119
26	BE	0.91	6/1571 (0.4%)	0.60	0/2113
27	BF	0.89	6/1434 (0.4%)	0.56	0/1926
28	BG	1.03	8/1343 (0.6%)	0.60	0/1816
29	BH	0.73	3/1121 (0.3%)	0.54	0/1515
30	BI	0.82	2/531 (0.4%)	0.55	0/709
31	BJ	1.09	7/1152 (0.6%)	0.62	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BK	1.08	5/955 (0.5%)	0.68	0/1279
33	BL	0.95	5/1062 (0.5%)	0.67	0/1413
34	BM	1.16	8/1081 (0.7%)	0.66	0/1443
35	BN	1.07	5/958 (0.5%)	0.68	0/1281
36	BO	0.81	2/910 (0.2%)	0.57	1/1219 (0.1%)
37	BP	0.99	3/929 (0.3%)	0.62	0/1242
38	BQ	0.93	0/960	0.58	0/1278
39	BR	0.91	2/829 (0.2%)	0.64	0/1107
40	BS	0.84	3/864 (0.3%)	0.60	0/1156
41	BT	0.79	1/744 (0.1%)	0.63	0/994
42	BU	0.96	3/787 (0.4%)	0.68	1/1051 (0.1%)
43	BV	1.06	4/766 (0.5%)	0.61	0/1025
44	BW	0.91	1/587 (0.2%)	0.63	0/776
45	BX	0.96	3/635 (0.5%)	0.66	1/848 (0.1%)
46	BY	0.55	0/502	0.56	0/667
47	BZ	0.97	2/453 (0.4%)	0.64	0/605
48	B0	0.89	2/450 (0.4%)	0.61	0/599
49	B1	1.09	2/421 (0.5%)	0.64	0/561
50	B2	0.97	1/380 (0.3%)	0.64	0/498
51	B3	1.21	4/513 (0.8%)	0.82	1/676 (0.1%)
52	B4	1.02	1/303 (0.3%)	0.67	0/397
53	B5	1.33	2/151 (1.3%)	0.81	0/205
54	B7	1.47	3/233 (1.3%)	2.72	14/358 (3.9%)
55	B8	1.87	57/1839 (3.1%)	2.96	169/2866 (5.9%)
56	B9	0.73	8/2806 (0.3%)	0.55	0/3778
All	All	1.72	3353/158589 (2.1%)	3.01	13021/236840 (5.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
51	B3	0	1
All	All	0	2

All (3353) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-22.33	1.28	1.53
22	BA	2449	U	C5-C6	18.12	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	O4'-C1'	16.77	1.63	1.41
55	B8	59	A	C6-N6	16.71	1.47	1.33
55	B8	58	A	C6-N6	16.69	1.47	1.33
55	B8	73	A	C6-N6	16.65	1.47	1.33
55	B8	51	A	C6-N6	16.61	1.47	1.33
55	B8	6	A	C6-N6	16.61	1.47	1.33
55	B8	42	A	C6-N6	16.57	1.47	1.33
54	B7	9	A	C6-N6	16.54	1.47	1.33
55	B8	26	A	C6-N6	16.50	1.47	1.33
55	B8	76	A	C6-N6	16.50	1.47	1.33
55	B8	14	A	C6-N6	16.45	1.47	1.33
55	B8	38	A	C6-N6	16.42	1.47	1.33
55	B8	66	A	C6-N6	16.40	1.47	1.33
55	B8	21	A	C6-N6	16.29	1.47	1.33
55	B8	41	A	C6-N6	16.14	1.46	1.33
55	B8	69	A	C6-N6	15.95	1.46	1.33
53	B5	24	PRO	N-CD	12.00	1.64	1.47
5	AE	57	PRO	N-CD	11.40	1.63	1.47
56	B9	267	PRO	N-CD	11.40	1.63	1.47
56	B9	6	PRO	N-CD	11.35	1.63	1.47
13	AM	115	PRO	N-CD	11.32	1.63	1.47
21	AU	2	PRO	N-CD	11.29	1.63	1.47
10	AJ	39	PRO	N-CD	11.23	1.63	1.47
6	AF	67	PRO	N-CD	11.19	1.63	1.47
10	AJ	79	PRO	N-CD	11.17	1.63	1.47
4	AD	139	PRO	N-CD	11.13	1.63	1.47
22	BA	892	A	C4'-O4'	-11.13	1.31	1.45
2	AB	158	PRO	N-CD	11.12	1.63	1.47
7	AG	2	PRO	N-CD	11.12	1.63	1.47
9	AI	23	PRO	N-CD	11.10	1.63	1.47
22	BA	2435	A	C5-C4	-11.09	1.30	1.38
42	BU	55	PRO	N-CD	11.07	1.63	1.47
4	AD	38	PRO	N-CD	11.05	1.63	1.47
9	AI	51	PRO	N-CD	11.04	1.63	1.47
27	BF	139	PRO	N-CD	11.01	1.63	1.47
56	B9	236	PRO	N-CD	11.01	1.63	1.47
6	AF	19	PRO	N-CD	11.00	1.63	1.47
10	AJ	41	PRO	N-CD	10.99	1.63	1.47
29	BH	38	PRO	N-CD	10.99	1.63	1.47
3	AC	17	PRO	N-CD	10.99	1.63	1.47
28	BG	8	PRO	N-CD	10.98	1.63	1.47
7	AG	16	PRO	N-CD	10.98	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	BU	48	PRO	N-CD	10.97	1.63	1.47
7	AG	14	PRO	N-CD	10.97	1.63	1.47
42	BU	50	PRO	N-CD	10.96	1.63	1.47
4	AD	186	PRO	N-CD	10.96	1.63	1.47
56	B9	44	PRO	N-CD	10.94	1.63	1.47
27	BF	109	PRO	N-CD	10.94	1.63	1.47
19	AS	30	PRO	N-CD	10.92	1.63	1.47
2	AB	48	PRO	N-CD	10.92	1.63	1.47
12	AL	122	PRO	N-CD	10.92	1.63	1.47
28	BG	112	PRO	N-CD	10.91	1.63	1.47
4	AD	168	PRO	N-CD	10.90	1.63	1.47
7	AG	71	PRO	N-CD	10.89	1.63	1.47
13	AM	10	PRO	N-CD	10.88	1.63	1.47
19	AS	9	PRO	N-CD	10.88	1.63	1.47
2	AB	182	PRO	N-CD	10.86	1.63	1.47
29	BH	118	PRO	N-CD	10.85	1.63	1.47
21	AU	11	PRO	N-CD	10.85	1.63	1.47
12	AL	22	PRO	N-CD	10.84	1.63	1.47
4	AD	46	PRO	N-CD	10.83	1.63	1.47
3	AC	60	PRO	N-CD	10.82	1.63	1.47
7	AG	93	PRO	N-CD	10.82	1.62	1.47
5	AE	150	PRO	N-CD	10.81	1.62	1.47
3	AC	73	PRO	N-CD	10.81	1.62	1.47
56	B9	224	PRO	N-CD	10.81	1.62	1.47
14	AN	94	PRO	N-CD	10.81	1.62	1.47
30	BI	42	PRO	N-CD	10.81	1.62	1.47
13	AM	112	PRO	N-CD	10.80	1.62	1.47
47	BZ	42	PRO	N-CD	10.79	1.62	1.47
49	B1	31	PRO	N-CD	10.79	1.62	1.47
6	AF	101	PRO	N-CD	10.78	1.62	1.47
28	BG	156	PRO	N-CD	10.76	1.62	1.47
32	BK	72	PRO	N-CD	10.75	1.62	1.47
12	AL	45	PRO	N-CD	10.74	1.62	1.47
2	AB	193	PRO	N-CD	10.74	1.62	1.47
12	AL	91	PRO	N-CD	10.74	1.62	1.47
24	BC	126	PRO	N-CD	10.74	1.62	1.47
12	AL	11	PRO	N-CD	10.73	1.62	1.47
19	AS	42	PRO	N-CD	10.73	1.62	1.47
13	AM	96	PRO	N-CD	10.73	1.62	1.47
3	AC	98	PRO	N-CD	10.72	1.62	1.47
22	BA	466	A	C5-C4	-10.70	1.31	1.38
24	BC	131	PRO	N-CD	10.70	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BM	72	PRO	N-CD	10.70	1.62	1.47
56	B9	50	PRO	N-CD	10.70	1.62	1.47
34	BM	4	PRO	N-CD	10.69	1.62	1.47
33	BL	119	PRO	N-CD	10.69	1.62	1.47
51	B3	2	PRO	N-CD	10.69	1.62	1.47
2	AB	29	PRO	N-CD	10.69	1.62	1.47
26	BE	129	PRO	N-CD	10.69	1.62	1.47
3	AC	174	PRO	N-CD	10.66	1.62	1.47
28	BG	126	PRO	N-CD	10.65	1.62	1.47
30	BI	7	PRO	N-CD	10.65	1.62	1.47
3	AC	109	PRO	N-CD	10.64	1.62	1.47
8	AH	93	PRO	N-CD	10.64	1.62	1.47
19	AS	59	PRO	N-CD	10.64	1.62	1.47
18	AR	41	PRO	N-CD	10.63	1.62	1.47
27	BF	176	PRO	N-CD	10.63	1.62	1.47
10	AJ	43	PRO	N-CD	10.63	1.62	1.47
8	AH	28	PRO	N-CD	10.62	1.62	1.47
19	AS	76	PRO	N-CD	10.62	1.62	1.47
7	AG	88	PRO	N-CD	10.62	1.62	1.47
22	BA	689	A	C5-C4	-10.62	1.31	1.38
56	B9	206	PRO	N-CD	10.61	1.62	1.47
14	AN	52	PRO	N-CD	10.61	1.62	1.47
43	BV	27	PRO	N-CD	10.60	1.62	1.47
9	AI	125	PRO	N-CD	10.59	1.62	1.47
6	AF	50	PRO	N-CD	10.59	1.62	1.47
4	AD	7	PRO	N-CD	10.59	1.62	1.47
24	BC	32	PRO	N-CD	10.58	1.62	1.47
28	BG	154	PRO	N-CD	10.57	1.62	1.47
11	AK	123	PRO	N-CD	10.57	1.62	1.47
8	AH	57	PRO	N-CD	10.55	1.62	1.47
16	AP	41	PRO	N-CD	10.55	1.62	1.47
2	AB	25	PRO	N-CD	10.55	1.62	1.47
14	AN	70	PRO	N-CD	10.55	1.62	1.47
32	BK	94	PRO	N-CD	10.54	1.62	1.47
35	BN	39	PRO	N-CD	10.53	1.62	1.47
6	AF	12	PRO	N-CD	10.52	1.62	1.47
29	BH	32	PRO	N-CD	10.52	1.62	1.47
36	BO	42	PRO	N-CD	10.51	1.62	1.47
17	AQ	66	PRO	N-CD	10.50	1.62	1.47
26	BE	177	PRO	N-CD	10.50	1.62	1.47
34	BM	77	PRO	N-CD	10.50	1.62	1.47
11	AK	89	PRO	N-CD	10.49	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	91	PRO	N-CD	10.49	1.62	1.47
43	BV	84	PRO	N-CD	10.49	1.62	1.47
28	BG	54	PRO	N-CD	10.48	1.62	1.47
39	BR	52	PRO	N-CD	10.48	1.62	1.47
5	AE	84	PRO	N-CD	10.48	1.62	1.47
2	AB	201	PRO	N-CD	10.48	1.62	1.47
17	AQ	32	PRO	N-CD	10.46	1.62	1.47
27	BF	84	PRO	N-CD	10.46	1.62	1.47
32	BK	48	PRO	N-CD	10.46	1.62	1.47
37	BP	18	PRO	N-CD	10.46	1.62	1.47
24	BC	218	PRO	N-CD	10.45	1.62	1.47
51	B3	63	PRO	N-CD	10.44	1.62	1.47
28	BG	118	PRO	N-CD	10.44	1.62	1.47
37	BP	22	PRO	N-CD	10.43	1.62	1.47
14	AN	57	PRO	N-CD	10.43	1.62	1.47
18	AR	69	PRO	N-CD	10.43	1.62	1.47
35	BN	109	PRO	N-CD	10.43	1.62	1.47
11	AK	115	PRO	N-CD	10.42	1.62	1.47
22	BA	2711	A	C5-C4	-10.42	1.31	1.38
11	AK	124	PRO	N-CD	10.42	1.62	1.47
25	BD	23	PRO	N-CD	10.41	1.62	1.47
24	BC	231	PRO	N-CD	10.41	1.62	1.47
24	BC	22	PRO	N-CD	10.41	1.62	1.47
5	AE	98	PRO	N-CD	10.40	1.62	1.47
21	AU	41	PRO	N-CD	10.40	1.62	1.47
48	B0	8	PRO	N-CD	10.40	1.62	1.47
24	BC	148	PRO	N-CD	10.39	1.62	1.47
35	BN	85	PRO	N-CD	10.39	1.62	1.47
8	AH	6	PRO	N-CD	10.37	1.62	1.47
28	BG	12	PRO	N-CD	10.37	1.62	1.47
43	BV	37	PRO	N-CD	10.37	1.62	1.47
20	AT	56	PRO	N-CD	10.36	1.62	1.47
22	BA	2542	A	C5-C4	-10.35	1.31	1.38
45	BX	12	PRO	N-CD	10.34	1.62	1.47
11	AK	117	PRO	N-CD	10.34	1.62	1.47
8	AH	81	PRO	N-CD	10.32	1.62	1.47
11	AK	60	PRO	N-CD	10.32	1.62	1.47
24	BC	8	PRO	N-CD	10.32	1.62	1.47
31	BJ	46	PRO	N-CD	10.31	1.62	1.47
47	BZ	18	PRO	N-CD	10.31	1.62	1.47
25	BD	152	PRO	N-CD	10.30	1.62	1.47
27	BF	29	PRO	N-CD	10.30	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	7	PRO	N-CD	10.29	1.62	1.47
25	BD	63	PRO	N-CD	10.29	1.62	1.47
10	AJ	55	PRO	N-CD	10.29	1.62	1.47
24	BC	227	PRO	N-CD	10.28	1.62	1.47
51	B3	46	PRO	N-CD	10.27	1.62	1.47
26	BE	89	PRO	N-CD	10.24	1.62	1.47
32	BK	120	PRO	N-CD	10.24	1.62	1.47
31	BJ	8	PRO	N-CD	10.24	1.62	1.47
49	B1	41	PRO	N-CD	10.24	1.62	1.47
22	BA	1783	A	C5-C4	-10.23	1.31	1.38
34	BM	125	PRO	N-CD	10.23	1.62	1.47
32	BK	102	PRO	N-CD	10.23	1.62	1.47
22	BA	2080	A	C5-C4	-10.21	1.31	1.38
41	BT	14	PRO	N-CD	10.20	1.62	1.47
22	BA	2600	A	C5-C4	-10.19	1.31	1.38
5	AE	133	PRO	N-CD	10.19	1.62	1.47
31	BJ	110	PRO	N-CD	10.18	1.62	1.47
24	BC	107	PRO	N-CD	10.18	1.62	1.47
43	BV	81	PRO	N-CD	10.17	1.62	1.47
34	BM	109	PRO	N-CD	10.14	1.62	1.47
40	BS	87	PRO	N-CD	10.14	1.62	1.47
31	BJ	137	PRO	N-CD	10.13	1.62	1.47
33	BL	8	PRO	N-CD	10.12	1.62	1.47
12	AL	42	PRO	N-CD	10.11	1.62	1.47
22	BA	1668	A	C5-C4	-10.11	1.31	1.38
22	BA	2052	A	C5-C4	-10.10	1.31	1.38
22	BA	2450	A	C5-C4	-10.10	1.31	1.38
12	AL	28	PRO	N-CD	10.09	1.61	1.47
25	BD	143	PRO	N-CD	10.09	1.61	1.47
37	BP	79	PRO	N-CD	10.08	1.61	1.47
27	BF	65	PRO	N-CD	10.07	1.61	1.47
44	BW	74	PRO	N-CD	10.07	1.61	1.47
52	B4	31	PRO	N-CD	10.06	1.61	1.47
22	BA	513	A	C5-C4	-10.06	1.31	1.38
35	BN	50	PRO	N-CD	10.04	1.61	1.47
40	BS	80	PRO	N-CD	10.04	1.61	1.47
24	BC	11	PRO	N-CD	10.04	1.61	1.47
24	BC	29	PRO	N-CD	10.03	1.61	1.47
50	B2	7	PRO	N-CD	10.03	1.61	1.47
34	BM	69	PRO	N-CD	10.01	1.61	1.47
36	BO	32	PRO	N-CD	10.01	1.61	1.47
22	BA	1571	A	C5-C4	-10.00	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BD	205	PRO	N-CD	10.00	1.61	1.47
26	BE	59	PRO	N-CD	10.00	1.61	1.47
25	BD	194	PRO	N-CD	9.94	1.61	1.47
16	AP	15	PRO	N-CD	9.92	1.61	1.47
24	BC	247	PRO	N-CD	9.91	1.61	1.47
22	BA	1264	A	C5-C4	-9.89	1.31	1.38
24	BC	85	PRO	N-CD	9.85	1.61	1.47
24	BC	75	PRO	N-CD	9.82	1.61	1.47
22	BA	1772	A	C5-C4	-9.79	1.31	1.38
22	BA	2358	A	C5-C4	-9.79	1.31	1.38
33	BL	56	PRO	N-CD	9.79	1.61	1.47
22	BA	2013	A	C5-C4	-9.76	1.31	1.38
24	BC	136	PRO	N-CD	9.74	1.61	1.47
22	BA	1028	A	C5-C4	-9.74	1.31	1.38
22	BA	2051	A	C5-C4	-9.74	1.31	1.38
22	BA	2328	A	C5-C4	-9.74	1.31	1.38
22	BA	2565	A	C5-C4	-9.72	1.31	1.38
31	BJ	113	PRO	N-CD	9.72	1.61	1.47
24	BC	244	PRO	N-CD	9.71	1.61	1.47
22	BA	2411	A	C5-C4	-9.70	1.31	1.38
22	BA	191	A	C5-C4	-9.70	1.31	1.38
22	BA	1901	A	C5-C4	-9.70	1.31	1.38
26	BE	76	PRO	N-CD	9.69	1.61	1.47
22	BA	1431	A	C5-C4	-9.67	1.31	1.38
22	BA	1129	A	C5-C4	-9.67	1.31	1.38
45	BX	31	PRO	N-CD	9.66	1.61	1.47
22	BA	2077	A	C5-C4	-9.66	1.31	1.38
22	BA	2090	A	C5-C4	-9.65	1.31	1.38
22	BA	631	A	C5-C4	-9.64	1.32	1.38
22	BA	207	A	C5-C4	-9.61	1.32	1.38
34	BM	98	PRO	N-CD	9.60	1.61	1.47
31	BJ	97	PRO	N-CD	9.59	1.61	1.47
22	BA	742	A	C5-C4	-9.58	1.32	1.38
22	BA	675	A	C5-C4	-9.56	1.32	1.38
22	BA	2726	A	C5-C4	-9.56	1.32	1.38
22	BA	2060	A	C5-C4	-9.56	1.32	1.38
22	BA	526	A	C5-C4	-9.55	1.32	1.38
22	BA	1353	A	C5-C4	-9.55	1.32	1.38
23	BB	99	A	C5-C4	-9.51	1.32	1.38
22	BA	2241	A	C5-C4	-9.49	1.32	1.38
22	BA	2740	A	C5-C4	-9.48	1.32	1.38
22	BA	449	A	C5-C4	-9.47	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1805	A	C5-C4	-9.46	1.32	1.38
22	BA	2541	A	C5-C4	-9.46	1.32	1.38
22	BA	2727	A	C5-C4	-9.45	1.32	1.38
22	BA	1787	A	C5-C4	-9.45	1.32	1.38
22	BA	2741	A	C5-C4	-9.43	1.32	1.38
22	BA	1378	A	C5-C4	-9.43	1.32	1.38
22	BA	833	A	C5-C4	-9.42	1.32	1.38
22	BA	1569	A	C5-C4	-9.42	1.32	1.38
22	BA	677	A	C5-C4	-9.42	1.32	1.38
22	BA	781	A	C5-C4	-9.39	1.32	1.38
22	BA	2461	A	C5-C4	-9.38	1.32	1.38
22	BA	1784	A	C5-C4	-9.38	1.32	1.38
22	BA	1328	A	C5-C4	-9.38	1.32	1.38
22	BA	743	A	C5-C4	-9.37	1.32	1.38
22	BA	2388	A	C5-C4	-9.37	1.32	1.38
22	BA	563	A	C5-C4	-9.37	1.32	1.38
22	BA	761	A	C5-C4	-9.37	1.32	1.38
22	BA	401	A	C5-C4	-9.37	1.32	1.38
22	BA	1854	A	C5-C4	-9.37	1.32	1.38
22	BA	582	A	C5-C4	-9.36	1.32	1.38
22	BA	2059	A	C5-C4	-9.35	1.32	1.38
22	BA	693	A	C5-C4	-9.35	1.32	1.38
22	BA	2721	A	C5-C4	-9.34	1.32	1.38
22	BA	2516	A	C5-C4	-9.34	1.32	1.38
22	BA	608	A	C5-C4	-9.34	1.32	1.38
22	BA	1987	A	C5-C4	-9.34	1.32	1.38
22	BA	203	A	C5-C4	-9.33	1.32	1.38
22	BA	1977	A	C5-C4	-9.33	1.32	1.38
22	BA	800	A	C5-C4	-9.33	1.32	1.38
33	BL	62	PRO	N-CD	9.33	1.60	1.47
22	BA	676	A	C5-C4	-9.32	1.32	1.38
22	BA	2725	A	C5-C4	-9.31	1.32	1.38
22	BA	2042	A	C5-C4	-9.30	1.32	1.38
22	BA	794	A	C5-C4	-9.29	1.32	1.38
22	BA	2682	A	C5-C4	-9.29	1.32	1.38
22	BA	2281	A	C5-C4	-9.27	1.32	1.38
22	BA	2821	A	C5-C4	-9.27	1.32	1.38
22	BA	2070	A	C5-C4	-9.26	1.32	1.38
22	BA	2883	A	C5-C4	-9.26	1.32	1.38
22	BA	2005	A	C5-C4	-9.25	1.32	1.38
22	BA	2033	A	C5-C4	-9.24	1.32	1.38
22	BA	1819	A	C5-C4	-9.21	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1678	A	C5-C4	-9.21	1.32	1.38
22	BA	586	A	C5-C4	-9.20	1.32	1.38
22	BA	2071	A	C5-C4	-9.20	1.32	1.38
22	BA	750	A	C5-C4	-9.19	1.32	1.38
22	BA	2020	A	C5-C4	-9.17	1.32	1.38
22	BA	1144	A	C5-C4	-9.17	1.32	1.38
22	BA	423	A	C5-C4	-9.16	1.32	1.38
22	BA	1226	A	C5-C4	-9.15	1.32	1.38
22	BA	2564	A	C5-C4	-9.15	1.32	1.38
22	BA	514	A	C5-C4	-9.14	1.32	1.38
22	BA	49	A	C5-C4	-9.12	1.32	1.38
22	BA	1960	A	C5-C4	-9.10	1.32	1.38
22	BA	1672	A	C5-C4	-9.10	1.32	1.38
22	BA	1853	A	C5-C4	-9.10	1.32	1.38
22	BA	119	A	C5-C4	-9.10	1.32	1.38
22	BA	1759	A	C5-C4	-9.10	1.32	1.38
22	BA	979	A	C5-C4	-9.09	1.32	1.38
22	BA	1802	A	C5-C4	-9.08	1.32	1.38
22	BA	1809	A	C5-C4	-9.07	1.32	1.38
22	BA	699	A	C5-C4	-9.04	1.32	1.38
22	BA	1213	A	C5-C4	-9.04	1.32	1.38
22	BA	1899	A	C5-C4	-9.04	1.32	1.38
22	BA	2425	A	C5-C4	-9.04	1.32	1.38
22	BA	2088	A	C5-C4	-9.03	1.32	1.38
22	BA	1165	A	C5-C4	-9.02	1.32	1.38
22	BA	2632	A	C5-C4	-9.02	1.32	1.38
22	BA	1260	A	C5-C4	-9.01	1.32	1.38
22	BA	204	A	C5-C4	-9.00	1.32	1.38
22	BA	2577	A	C5-C4	-8.99	1.32	1.38
22	BA	309	A	C5-C4	-8.97	1.32	1.38
22	BA	1970	A	C5-C4	-8.96	1.32	1.38
22	BA	825	A	C5-C4	-8.96	1.32	1.38
22	BA	1637	A	C5-C4	-8.96	1.32	1.38
22	BA	1596	A	C5-C4	-8.95	1.32	1.38
22	BA	501	A	C5-C4	-8.94	1.32	1.38
22	BA	1000	A	C5-C4	-8.94	1.32	1.38
22	BA	1269	A	C5-C4	-8.93	1.32	1.38
22	BA	1677	A	C5-C4	-8.92	1.32	1.38
22	BA	988	A	C5-C4	-8.92	1.32	1.38
22	BA	756	A	C5-C4	-8.91	1.32	1.38
22	BA	1354	A	C5-C4	-8.90	1.32	1.38
22	BA	1385	A	C5-C4	-8.90	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1570	A	C5-C4	-8.90	1.32	1.38
22	BA	1268	A	C5-C4	-8.90	1.32	1.38
22	BA	52	A	C5-C4	-8.89	1.32	1.38
22	BA	1155	A	C5-C4	-8.89	1.32	1.38
22	BA	2589	A	C5-C4	-8.89	1.32	1.38
22	BA	1794	A	C5-C4	-8.88	1.32	1.38
22	BA	2829	A	C5-C4	-8.88	1.32	1.38
22	BA	447	A	C5-C4	-8.88	1.32	1.38
22	BA	1143	A	C5-C4	-8.88	1.32	1.38
22	BA	668	A	C5-C4	-8.87	1.32	1.38
22	BA	1342	A	C5-C4	-8.86	1.32	1.38
22	BA	2518	A	C5-C4	-8.86	1.32	1.38
22	BA	1548	A	C5-C4	-8.85	1.32	1.38
22	BA	1287	A	C5-C4	-8.85	1.32	1.38
22	BA	439	A	C5-C4	-8.84	1.32	1.38
22	BA	2837	A	C5-C4	-8.84	1.32	1.38
25	BD	152	PRO	N-CA	-8.83	1.32	1.47
22	BA	479	A	C5-C4	-8.83	1.32	1.38
22	BA	2054	A	C5-C4	-8.83	1.32	1.38
22	BA	457	A	C5-C4	-8.82	1.32	1.38
22	BA	196	A	C5-C4	-8.81	1.32	1.38
22	BA	233	A	C5-C4	-8.81	1.32	1.38
22	BA	1254	A	C5-C4	-8.80	1.32	1.38
22	BA	1189	A	C5-C4	-8.80	1.32	1.38
22	BA	1265	A	C5-C4	-8.80	1.32	1.38
22	BA	1572	A	C5-C4	-8.80	1.32	1.38
22	BA	751	A	C5-C4	-8.80	1.32	1.38
22	BA	792	A	C5-C4	-8.80	1.32	1.38
22	BA	1308	A	C5-C4	-8.80	1.32	1.38
22	BA	1952	A	C5-C4	-8.79	1.32	1.38
22	BA	2270	A	C5-C4	-8.79	1.32	1.38
22	BA	522	A	C5-C4	-8.79	1.32	1.38
22	BA	981	A	C5-C4	-8.79	1.32	1.38
22	BA	1286	A	C5-C4	-8.79	1.32	1.38
22	BA	983	A	C5-C4	-8.78	1.32	1.38
22	BA	2547	A	C5-C4	-8.78	1.32	1.38
22	BA	1652	A	C5-C4	-8.77	1.32	1.38
22	BA	6	A	C5-C4	-8.77	1.32	1.38
22	BA	1010	A	C5-C4	-8.77	1.32	1.38
22	BA	2031	A	C5-C4	-8.77	1.32	1.38
22	BA	1366	A	C5-C4	-8.75	1.32	1.38
22	BA	53	A	C5-C4	-8.75	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2037	A	C5-C4	-8.75	1.32	1.38
22	BA	2434	A	C5-C4	-8.74	1.32	1.38
22	BA	1803	A	C5-C4	-8.74	1.32	1.38
22	BA	1815	A	C5-C4	-8.74	1.32	1.38
22	BA	222	A	C5-C4	-8.73	1.32	1.38
22	BA	980	A	C5-C4	-8.72	1.32	1.38
22	BA	1711	A	C5-C4	-8.72	1.32	1.38
22	BA	1655	A	C5-C4	-8.72	1.32	1.38
22	BA	2860	A	C5-C4	-8.72	1.32	1.38
22	BA	412	A	C5-C4	-8.72	1.32	1.38
22	BA	2381	A	C5-C4	-8.71	1.32	1.38
22	BA	2598	A	C5-C4	-8.71	1.32	1.38
22	BA	1632	A	C5-C4	-8.69	1.32	1.38
22	BA	1032	A	C5-C4	-8.68	1.32	1.38
22	BA	1821	A	C5-C4	-8.68	1.32	1.38
22	BA	2764	A	C5-C4	-8.68	1.32	1.38
22	BA	2227	A	C5-C4	-8.68	1.32	1.38
22	BA	1700	A	C5-C4	-8.66	1.32	1.38
22	BA	216	A	C5-C4	-8.65	1.32	1.38
22	BA	2247	A	C5-C4	-8.65	1.32	1.38
22	BA	73	A	C5-C4	-8.65	1.32	1.38
22	BA	2459	A	C5-C4	-8.65	1.32	1.38
22	BA	1791	A	C5-C4	-8.64	1.32	1.38
22	BA	89	A	C5-C4	-8.63	1.32	1.38
22	BA	1373	A	C5-C4	-8.62	1.32	1.38
22	BA	1650	A	C5-C4	-8.62	1.32	1.38
22	BA	727	A	C5-C4	-8.62	1.32	1.38
22	BA	661	A	C5-C4	-8.61	1.32	1.38
22	BA	749	A	C5-C4	-8.61	1.32	1.38
22	BA	1156	A	C5-C4	-8.60	1.32	1.38
22	BA	920	A	C5-C4	-8.59	1.32	1.38
22	BA	602	A	C5-C4	-8.58	1.32	1.38
22	BA	972	A	C5-C4	-8.58	1.32	1.38
22	BA	1566	A	C5-C4	-8.58	1.32	1.38
22	BA	1419	A	C5-C4	-8.58	1.32	1.38
22	BA	943	A	C5-C4	-8.58	1.32	1.38
22	BA	2850	A	C5-C4	-8.58	1.32	1.38
22	BA	1754	A	C5-C4	-8.57	1.32	1.38
22	BA	1009	A	C5-C4	-8.57	1.32	1.38
22	BA	2665	A	C5-C4	-8.56	1.32	1.38
22	BA	1755	A	C5-C4	-8.56	1.32	1.38
22	BA	2388	A	N7-C5	-8.56	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	477	A	C5-C4	-8.55	1.32	1.38
22	BA	730	A	C5-C4	-8.55	1.32	1.38
22	BA	2412	A	C5-C4	-8.55	1.32	1.38
22	BA	2823	A	C5-C4	-8.55	1.32	1.38
22	BA	670	A	C5-C4	-8.55	1.32	1.38
22	BA	2340	A	C5-C4	-8.55	1.32	1.38
22	BA	863	A	C5-C4	-8.55	1.32	1.38
22	BA	2614	A	C5-C4	-8.55	1.32	1.38
1	AA	1513	A	C5-C4	-8.54	1.32	1.38
22	BA	1978	A	C5-C4	-8.54	1.32	1.38
22	BA	1665	A	C5-C4	-8.54	1.32	1.38
22	BA	1829	A	C5-C4	-8.54	1.32	1.38
22	BA	1275	A	C5-C4	-8.54	1.32	1.38
22	BA	2679	A	C5-C4	-8.54	1.32	1.38
22	BA	231	A	C5-C4	-8.54	1.32	1.38
22	BA	422	A	C5-C4	-8.53	1.32	1.38
22	BA	2386	A	C5-C4	-8.53	1.32	1.38
22	BA	2453	A	C5-C4	-8.53	1.32	1.38
22	BA	432	A	C5-C4	-8.52	1.32	1.38
22	BA	821	A	C5-C4	-8.52	1.32	1.38
22	BA	861	A	C5-C4	-8.52	1.32	1.38
22	BA	2766	A	C5-C4	-8.52	1.32	1.38
22	BA	2675	A	C5-C4	-8.52	1.32	1.38
22	BA	788	A	C5-C4	-8.51	1.32	1.38
22	BA	2418	A	C5-C4	-8.51	1.32	1.38
22	BA	176	A	C5-C4	-8.51	1.32	1.38
22	BA	2335	A	C5-C4	-8.50	1.32	1.38
1	AA	675	A	C5-C4	-8.50	1.32	1.38
22	BA	532	A	C5-C4	-8.49	1.32	1.38
22	BA	19	A	C5-C4	-8.48	1.32	1.38
22	BA	1384	A	C5-C4	-8.48	1.32	1.38
22	BA	310	A	C5-C4	-8.48	1.32	1.38
22	BA	262	A	C5-C4	-8.48	1.32	1.38
22	BA	734	A	C5-C4	-8.47	1.32	1.38
22	BA	2058	A	C5-C4	-8.47	1.32	1.38
22	BA	453	A	C5-C4	-8.47	1.32	1.38
22	BA	1194	A	C5-C4	-8.46	1.32	1.38
22	BA	1900	A	C5-C4	-8.46	1.32	1.38
22	BA	199	A	C5-C4	-8.45	1.32	1.38
22	BA	2019	A	C5-C4	-8.45	1.32	1.38
22	BA	2288	A	C5-C4	-8.45	1.32	1.38
22	BA	990	A	C5-C4	-8.45	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	804	A	C5-C4	-8.45	1.32	1.38
22	BA	38	A	C5-C4	-8.44	1.32	1.38
22	BA	1133	A	C5-C4	-8.44	1.32	1.38
22	BA	454	A	C5-C4	-8.43	1.32	1.38
22	BA	1626	A	C5-C4	-8.43	1.32	1.38
22	BA	917	A	C5-C4	-8.43	1.32	1.38
22	BA	1247	A	C5-C4	-8.43	1.32	1.38
1	AA	781	A	C5-C4	-8.42	1.32	1.38
22	BA	1253	A	C5-C4	-8.42	1.32	1.38
23	BB	104	A	C5-C4	-8.42	1.32	1.38
22	BA	126	A	C5-C4	-8.41	1.32	1.38
22	BA	1142	A	C5-C4	-8.41	1.32	1.38
22	BA	371	A	C5-C4	-8.41	1.32	1.38
22	BA	1966	A	C5-C4	-8.40	1.32	1.38
22	BA	1608	A	C5-C4	-8.40	1.32	1.38
22	BA	1953	A	C5-C4	-8.40	1.32	1.38
22	BA	789	A	C5-C4	-8.40	1.32	1.38
22	BA	2468	A	C5-C4	-8.40	1.32	1.38
22	BA	945	A	C5-C4	-8.39	1.32	1.38
22	BA	1928	A	C5-C4	-8.39	1.32	1.38
22	BA	2015	A	C5-C4	-8.39	1.32	1.38
22	BA	430	A	C5-C4	-8.39	1.32	1.38
22	BA	1127	A	C5-C4	-8.39	1.32	1.38
22	BA	2781	A	C5-C4	-8.39	1.32	1.38
22	BA	1773	A	C5-C4	-8.38	1.32	1.38
22	BA	599	A	C5-C4	-8.38	1.32	1.38
22	BA	1789	A	C5-C4	-8.38	1.32	1.38
23	BB	78	A	C5-C4	-8.38	1.32	1.38
22	BA	2278	A	C5-C4	-8.38	1.32	1.38
22	BA	2873	A	C5-C4	-8.37	1.32	1.38
22	BA	118	A	C5-C4	-8.37	1.32	1.38
1	AA	766	A	C5-C4	-8.37	1.32	1.38
22	BA	1151	A	C5-C4	-8.36	1.32	1.38
22	BA	2014	A	C5-C4	-8.36	1.32	1.38
1	AA	777	A	C5-C4	-8.36	1.32	1.38
22	BA	2469	A	C5-C4	-8.36	1.32	1.38
1	AA	792	A	C5-C4	-8.35	1.32	1.38
22	BA	221	A	C5-C4	-8.35	1.32	1.38
22	BA	1749	A	C5-C4	-8.35	1.32	1.38
22	BA	575	A	C5-C4	-8.35	1.32	1.38
22	BA	2369	A	C5-C4	-8.35	1.32	1.38
22	BA	2560	A	C5-C4	-8.35	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2750	A	C5-C4	-8.34	1.32	1.38
22	BA	637	A	C5-C4	-8.34	1.32	1.38
22	BA	1029	A	C5-C4	-8.34	1.32	1.38
22	BA	415	A	C5-C4	-8.33	1.32	1.38
22	BA	1664	A	C5-C4	-8.33	1.32	1.38
22	BA	947	A	C5-C4	-8.33	1.32	1.38
22	BA	2268	A	C5-C4	-8.33	1.32	1.38
1	AA	814	A	C5-C4	-8.33	1.32	1.38
22	BA	56	A	C5-C4	-8.33	1.32	1.38
22	BA	1609	A	C5-C4	-8.33	1.32	1.38
22	BA	1439	A	C5-C4	-8.32	1.32	1.38
22	BA	2376	A	C5-C4	-8.32	1.32	1.38
22	BA	1470	A	C5-C4	-8.32	1.32	1.38
22	BA	471	A	C5-C4	-8.31	1.32	1.38
22	BA	941	A	C5-C4	-8.31	1.32	1.38
22	BA	685	A	C5-C4	-8.31	1.32	1.38
22	BA	1981	A	C5-C4	-8.31	1.32	1.38
22	BA	1403	A	C5-C4	-8.30	1.32	1.38
22	BA	195	A	C5-C4	-8.30	1.32	1.38
22	BA	1214	A	C5-C4	-8.30	1.32	1.38
22	BA	984	A	C5-C4	-8.29	1.32	1.38
22	BA	1126	A	C5-C4	-8.29	1.32	1.38
22	BA	2003	A	C5-C4	-8.29	1.32	1.38
1	AA	845	A	C8-N7	8.29	1.37	1.31
22	BA	627	A	C5-C4	-8.29	1.32	1.38
7	AG	2	PRO	N-CA	-8.28	1.33	1.47
22	BA	735	A	C5-C4	-8.28	1.32	1.38
22	BA	2062	A	C5-C4	-8.28	1.32	1.38
22	BA	819	A	C5-C4	-8.27	1.32	1.38
22	BA	2706	A	C5-C4	-8.27	1.32	1.38
22	BA	227	A	C5-C4	-8.26	1.32	1.38
22	BA	1932	A	C5-C4	-8.26	1.32	1.38
22	BA	574	A	C5-C4	-8.26	1.32	1.38
22	BA	2765	A	C5-C4	-8.25	1.32	1.38
22	BA	975	A	C5-C4	-8.25	1.32	1.38
22	BA	2639	A	C5-C4	-8.24	1.32	1.38
22	BA	2448	A	C5-C4	-8.24	1.32	1.38
22	BA	2451	A	C5-C4	-8.24	1.32	1.38
22	BA	2497	A	C5-C4	-8.24	1.32	1.38
22	BA	1552	A	C5-C4	-8.23	1.32	1.38
22	BA	1802	A	N7-C5	-8.23	1.34	1.39
1	AA	665	A	C5-C4	-8.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2433	A	C5-C4	-8.23	1.32	1.38
22	BA	1469	A	C5-C4	-8.22	1.32	1.38
22	BA	632	A	C5-C4	-8.22	1.32	1.38
22	BA	705	A	C5-C4	-8.22	1.32	1.38
22	BA	2471	A	C5-C4	-8.22	1.32	1.38
22	BA	2899	A	C5-C4	-8.22	1.32	1.38
1	AA	1499	A	C5-C4	-8.21	1.33	1.38
1	AA	1433	A	C5-C4	-8.20	1.33	1.38
22	BA	844	A	C5-C4	-8.19	1.33	1.38
39	BR	52	PRO	N-CA	-8.19	1.33	1.47
1	AA	780	A	C5-C4	-8.19	1.33	1.38
22	BA	497	A	C5-C4	-8.19	1.33	1.38
22	BA	1701	A	C5-C4	-8.19	1.33	1.38
22	BA	1001	A	C5-C4	-8.19	1.33	1.38
1	AA	802	A	C5-C4	-8.19	1.33	1.38
22	BA	1919	A	C5-C4	-8.18	1.33	1.38
22	BA	1336	A	C5-C4	-8.18	1.33	1.38
22	BA	1810	A	C5-C4	-8.18	1.33	1.38
22	BA	2225	A	C5-C4	-8.17	1.33	1.38
51	B3	2	PRO	N-CA	-8.17	1.33	1.47
22	BA	515	A	C5-C4	-8.17	1.33	1.38
22	BA	960	A	C5-C4	-8.17	1.33	1.38
22	BA	1365	A	C5-C4	-8.17	1.33	1.38
1	AA	1429	A	C5-C4	-8.16	1.33	1.38
1	AA	784	A	C5-C4	-8.16	1.33	1.38
12	AL	45	PRO	N-CA	-8.15	1.33	1.47
22	BA	1549	A	C5-C4	-8.15	1.33	1.38
22	BA	2590	A	C5-C4	-8.15	1.33	1.38
22	BA	320	A	C5-C4	-8.15	1.33	1.38
22	BA	592	A	C5-C4	-8.15	1.33	1.38
22	BA	2212	A	C5-C4	-8.15	1.33	1.38
22	BA	1551	A	C5-C4	-8.13	1.33	1.38
22	BA	1936	A	C5-C4	-8.13	1.33	1.38
22	BA	541	A	C5-C4	-8.13	1.33	1.38
55	B8	76	A	C8-N7	8.13	1.37	1.31
22	BA	2778	A	C5-C4	-8.13	1.33	1.38
22	BA	2336	A	C5-C4	-8.13	1.33	1.38
22	BA	503	A	C5-C4	-8.12	1.33	1.38
22	BA	1690	A	C5-C4	-8.12	1.33	1.38
13	AM	115	PRO	N-CA	-8.12	1.33	1.47
22	BA	256	A	C5-C4	-8.12	1.33	1.38
22	BA	1610	A	C5-C4	-8.12	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	330	A	C5-C4	-8.11	1.33	1.38
22	BA	2392	A	C5-C4	-8.11	1.33	1.38
22	BA	621	A	C5-C4	-8.11	1.33	1.38
22	BA	226	A	C5-C4	-8.10	1.33	1.38
22	BA	1679	A	C5-C4	-8.10	1.33	1.38
22	BA	1395	A	C5-C4	-8.09	1.33	1.38
22	BA	2094	A	C5-C4	-8.09	1.33	1.38
22	BA	74	A	C5-C4	-8.09	1.33	1.38
22	BA	332	A	C5-C4	-8.09	1.33	1.38
22	BA	1274	A	C5-C4	-8.08	1.33	1.38
22	BA	2273	A	C5-C4	-8.08	1.33	1.38
22	BA	2513	A	C5-C4	-8.07	1.33	1.38
22	BA	572	A	C5-C4	-8.07	1.33	1.38
22	BA	1244	A	C5-C4	-8.07	1.33	1.38
22	BA	706	A	C5-C4	-8.07	1.33	1.38
21	AU	2	PRO	N-CA	-8.06	1.33	1.47
22	BA	191	A	N7-C5	-8.06	1.34	1.39
1	AA	900	A	C5-C4	-8.06	1.33	1.38
22	BA	217	A	C5-C4	-8.05	1.33	1.38
1	AA	1483	A	C5-C4	-8.04	1.33	1.38
22	BA	633	A	C5-C4	-8.04	1.33	1.38
22	BA	959	A	C5-C4	-8.04	1.33	1.38
22	BA	1998	A	C5-C4	-8.04	1.33	1.38
22	BA	927	A	C5-C4	-8.03	1.33	1.38
22	BA	1285	A	C5-C4	-8.03	1.33	1.38
22	BA	2516	A	N7-C5	-8.03	1.34	1.39
1	AA	364	A	C5-C4	-8.03	1.33	1.38
22	BA	909	A	C5-C4	-8.02	1.33	1.38
22	BA	739	A	C5-C4	-8.02	1.33	1.38
22	BA	1889	A	C5-C4	-8.02	1.33	1.38
22	BA	2284	A	C5-C4	-8.02	1.33	1.38
1	AA	715	A	C5-C4	-8.01	1.33	1.38
22	BA	1301	A	C5-C4	-8.01	1.33	1.38
22	BA	1347	A	C5-C4	-8.01	1.33	1.38
22	BA	1634	A	C5-C4	-8.01	1.33	1.38
1	AA	1476	A	C5-C4	-8.00	1.33	1.38
22	BA	1698	A	C5-C4	-8.00	1.33	1.38
22	BA	529	A	C5-C4	-7.99	1.33	1.38
22	BA	1392	A	C5-C4	-7.99	1.33	1.38
22	BA	1387	A	C5-C4	-7.99	1.33	1.38
22	BA	2266	A	C5-C4	-7.99	1.33	1.38
1	AA	1021	A	C8-N7	7.98	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1262	A	C5-C4	-7.98	1.33	1.38
22	BA	2826	A	C5-C4	-7.98	1.33	1.38
22	BA	2009	A	C5-C4	-7.98	1.33	1.38
1	AA	1502	A	C5-C4	-7.97	1.33	1.38
1	AA	579	A	C5-C4	-7.96	1.33	1.38
1	AA	320	A	C5-C4	-7.96	1.33	1.38
22	BA	538	A	C5-C4	-7.96	1.33	1.38
22	BA	213	A	C5-C4	-7.96	1.33	1.38
22	BA	1246	A	C5-C4	-7.95	1.33	1.38
1	AA	1431	A	C5-C4	-7.95	1.33	1.38
22	BA	460	A	C5-C4	-7.94	1.33	1.38
22	BA	324	A	C5-C4	-7.94	1.33	1.38
22	BA	13	A	C5-C4	-7.94	1.33	1.38
22	BA	2170	A	C8-N7	7.93	1.37	1.31
22	BA	1937	A	C5-C4	-7.93	1.33	1.38
1	AA	1408	A	C5-C4	-7.93	1.33	1.38
22	BA	127	A	C5-C4	-7.93	1.33	1.38
22	BA	2635	A	C5-C4	-7.92	1.33	1.38
22	BA	2734	A	C5-C4	-7.92	1.33	1.38
1	AA	1213	A	C8-N7	7.92	1.37	1.31
22	BA	1393	A	C5-C4	-7.92	1.33	1.38
22	BA	402	A	C5-C4	-7.92	1.33	1.38
22	BA	2333	A	C5-C4	-7.91	1.33	1.38
1	AA	915	A	C5-C4	-7.91	1.33	1.38
22	BA	910	A	C5-C4	-7.91	1.33	1.38
22	BA	1327	A	C5-C4	-7.91	1.33	1.38
22	BA	2738	A	C5-C4	-7.91	1.33	1.38
22	BA	84	A	C5-C4	-7.90	1.33	1.38
1	AA	816	A	C5-C4	-7.90	1.33	1.38
22	BA	5	A	C5-C4	-7.90	1.33	1.38
22	BA	1433	A	C5-C4	-7.89	1.33	1.38
22	BA	1553	A	C5-C4	-7.89	1.33	1.38
22	BA	2287	A	C5-C4	-7.89	1.33	1.38
22	BA	14	A	C5-C4	-7.89	1.33	1.38
22	BA	28	A	C5-C4	-7.88	1.33	1.38
22	BA	1284	A	C5-C4	-7.88	1.33	1.38
22	BA	1525	A	C5-C4	-7.88	1.33	1.38
10	AJ	39	PRO	N-CA	-7.88	1.33	1.47
22	BA	2748	A	C5-C4	-7.88	1.33	1.38
22	BA	111	A	C5-C4	-7.88	1.33	1.38
22	BA	590	A	C5-C4	-7.88	1.33	1.38
1	AA	19	A	C5-C4	-7.87	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	219	A	C5-C4	-7.87	1.33	1.38
1	AA	1036	A	C8-N7	7.87	1.37	1.31
1	AA	1428	A	C5-C4	-7.87	1.33	1.38
22	BA	973	A	C5-C4	-7.87	1.33	1.38
22	BA	2851	A	C5-C4	-7.86	1.33	1.38
22	BA	2426	A	C5-C4	-7.86	1.33	1.38
1	AA	478	A	C8-N7	7.85	1.37	1.31
1	AA	759	A	C5-C4	-7.85	1.33	1.38
22	BA	1787	A	N7-C5	-7.85	1.34	1.39
22	BA	2700	A	C5-C4	-7.85	1.33	1.38
22	BA	1147	A	C5-C4	-7.84	1.33	1.38
22	BA	936	A	C5-C4	-7.83	1.33	1.38
22	BA	996	A	C5-C4	-7.83	1.33	1.38
22	BA	911	A	C5-C4	-7.83	1.33	1.38
22	BA	1630	A	C5-C4	-7.83	1.33	1.38
22	BA	666	A	C5-C4	-7.83	1.33	1.38
22	BA	83	A	C5-C4	-7.83	1.33	1.38
22	BA	1287	A	N7-C5	-7.83	1.34	1.39
22	BA	1535	A	C8-N7	7.83	1.37	1.31
22	BA	1717	A	C5-C4	-7.82	1.33	1.38
22	BA	294	A	C5-C4	-7.82	1.33	1.38
1	AA	583	A	C5-C4	-7.82	1.33	1.38
1	AA	68	G	N7-C5	-7.81	1.34	1.39
22	BA	1427	A	C5-C4	-7.81	1.33	1.38
22	BA	152	A	C5-C4	-7.80	1.33	1.38
22	BA	2327	A	C5-C4	-7.80	1.33	1.38
22	BA	1597	A	C5-C4	-7.80	1.33	1.38
22	BA	64	A	C5-C4	-7.80	1.33	1.38
22	BA	2274	A	C5-C4	-7.80	1.33	1.38
1	AA	77	A	C8-N7	7.80	1.37	1.31
22	BA	2352	A	C5-C4	-7.80	1.33	1.38
22	BA	1969	A	N7-C5	-7.80	1.34	1.39
22	BA	1616	A	C5-C4	-7.79	1.33	1.38
1	AA	782	A	C5-C4	-7.79	1.33	1.38
1	AA	919	A	C5-C4	-7.79	1.33	1.38
22	BA	802	A	N7-C5	-7.79	1.34	1.39
22	BA	2199	A	C5-C4	-7.79	1.33	1.38
22	BA	2657	A	C5-C4	-7.79	1.33	1.38
22	BA	478	A	C5-C4	-7.78	1.33	1.38
22	BA	1272	A	C5-C4	-7.78	1.33	1.38
22	BA	2082	A	C5-C4	-7.78	1.33	1.38
23	BB	108	A	C5-C4	-7.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2482	A	C5-C4	-7.78	1.33	1.38
22	BA	2893	A	C5-C4	-7.78	1.33	1.38
1	AA	16	A	C5-C4	-7.77	1.33	1.38
22	BA	502	A	C5-C4	-7.77	1.33	1.38
1	AA	71	A	C8-N7	7.77	1.36	1.31
23	BB	94	A	C5-C4	-7.76	1.33	1.38
22	BA	311	A	C5-C4	-7.76	1.33	1.38
23	BB	115	A	C5-C4	-7.76	1.33	1.38
22	BA	2810	A	C5-C4	-7.76	1.33	1.38
22	BA	1614	A	C5-C4	-7.75	1.33	1.38
22	BA	483	A	C5-C4	-7.75	1.33	1.38
22	BA	845	A	C5-C4	-7.75	1.33	1.38
23	BB	109	A	C5-C4	-7.74	1.33	1.38
22	BA	223	A	C5-C4	-7.74	1.33	1.38
22	BA	1367	A	C5-C4	-7.74	1.33	1.38
22	BA	918	A	C5-C4	-7.74	1.33	1.38
22	BA	644	A	C5-C4	-7.73	1.33	1.38
22	BA	802	A	C5-C4	-7.73	1.33	1.38
22	BA	2758	A	C5-C4	-7.73	1.33	1.38
22	BA	384	A	C5-C4	-7.73	1.33	1.38
22	BA	131	A	C5-C4	-7.73	1.33	1.38
22	BA	1014	A	C5-C4	-7.73	1.33	1.38
22	BA	1328	A	N7-C5	-7.72	1.34	1.39
1	AA	10	A	C5-C4	-7.72	1.33	1.38
1	AA	353	A	C5-C4	-7.72	1.33	1.38
22	BA	2163	A	C8-N7	7.71	1.36	1.31
22	BA	2776	A	C5-C4	-7.71	1.33	1.38
22	BA	1969	A	C5-C4	-7.71	1.33	1.38
22	BA	2267	A	C5-C4	-7.71	1.33	1.38
22	BA	2476	A	C5-C4	-7.71	1.33	1.38
22	BA	1545	A	C5-C4	-7.71	1.33	1.38
22	BA	1927	A	C5-C4	-7.71	1.33	1.38
22	BA	2814	A	C5-C4	-7.69	1.33	1.38
1	AA	1042	A	C8-N7	7.69	1.36	1.31
22	BA	753	A	C5-C4	-7.68	1.33	1.38
22	BA	428	A	C5-C4	-7.68	1.33	1.38
1	AA	865	A	C5-C4	-7.68	1.33	1.38
22	BA	643	A	C5-C4	-7.68	1.33	1.38
1	AA	1022	A	C8-N7	7.67	1.36	1.31
22	BA	2119	A	C8-N7	7.67	1.36	1.31
22	BA	2572	A	C5-C4	-7.67	1.33	1.38
22	BA	42	A	C5-C4	-7.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1096	A	C8-N7	7.66	1.36	1.31
22	BA	1689	A	C5-C4	-7.66	1.33	1.38
22	BA	1008	A	C5-C4	-7.66	1.33	1.38
22	BA	197	A	C5-C4	-7.66	1.33	1.38
56	B9	6	PRO	N-CA	-7.66	1.34	1.47
1	AA	787	A	C5-C4	-7.66	1.33	1.38
22	BA	195	A	C8-N7	7.65	1.36	1.31
55	B8	73	A	C8-N7	7.65	1.36	1.31
1	AA	559	A	C5-C4	-7.65	1.33	1.38
22	BA	2887	A	C5-C4	-7.65	1.33	1.38
22	BA	2670	A	C5-C4	-7.65	1.33	1.38
22	BA	190	A	C5-C4	-7.65	1.33	1.38
22	BA	1641	A	C5-C4	-7.65	1.33	1.38
1	AA	119	A	C5-C4	-7.64	1.33	1.38
22	BA	1276	A	C5-C4	-7.63	1.33	1.38
22	BA	609	A	C5-C4	-7.63	1.33	1.38
22	BA	2135	A	C8-N7	7.63	1.36	1.31
22	BA	2497	A	N7-C5	-7.63	1.34	1.39
22	BA	928	A	C5-C4	-7.62	1.33	1.38
22	BA	1890	A	C5-C4	-7.62	1.33	1.38
22	BA	820	A	C5-C4	-7.62	1.33	1.38
22	BA	2158	A	C8-N7	7.62	1.36	1.31
22	BA	2531	A	C5-C4	-7.62	1.33	1.38
22	BA	547	A	C8-N7	7.62	1.36	1.31
22	BA	1522	A	C5-C4	-7.62	1.33	1.38
1	AA	1145	A	C8-N7	7.61	1.36	1.31
22	BA	1786	A	C5-C4	-7.61	1.33	1.38
1	AA	327	A	C5-C4	-7.61	1.33	1.38
22	BA	2459	A	N7-C5	-7.61	1.34	1.39
22	BA	764	A	C5-C4	-7.61	1.33	1.38
1	AA	321	A	C5-C4	-7.61	1.33	1.38
22	BA	782	A	C5-C4	-7.60	1.33	1.38
1	AA	116	A	C5-C4	-7.60	1.33	1.38
22	BA	1086	A	C8-N7	7.59	1.36	1.31
22	BA	1095	A	C8-N7	7.59	1.36	1.31
1	AA	349	A	C5-C4	-7.59	1.33	1.38
22	BA	1237	A	C5-C4	-7.59	1.33	1.38
22	BA	2013	A	N7-C5	-7.59	1.34	1.39
1	AA	81	A	C8-N7	7.59	1.36	1.31
1	AA	1500	A	C5-C4	-7.58	1.33	1.38
22	BA	1359	A	C5-C4	-7.58	1.33	1.38
22	BA	181	A	C5-C4	-7.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1302	A	C5-C4	-7.58	1.33	1.38
1	AA	913	A	C5-C4	-7.58	1.33	1.38
1	AA	1413	A	C5-C4	-7.58	1.33	1.38
22	BA	10	A	C5-C4	-7.58	1.33	1.38
1	AA	572	A	C5-C4	-7.57	1.33	1.38
22	BA	340	A	C5-C4	-7.57	1.33	1.38
22	BA	1129	A	N7-C5	-7.57	1.34	1.39
22	BA	382	A	C5-C4	-7.56	1.33	1.38
22	BA	613	A	C8-N7	7.56	1.36	1.31
22	BA	52	A	N7-C5	-7.56	1.34	1.39
1	AA	74	A	C8-N7	7.55	1.36	1.31
1	AA	356	A	C5-C4	-7.55	1.33	1.38
22	BA	1204	A	C5-C4	-7.54	1.33	1.38
22	BA	2205	A	C5-C4	-7.54	1.33	1.38
1	AA	794	A	C5-C4	-7.53	1.33	1.38
22	BA	2872	A	C5-C4	-7.53	1.33	1.38
22	BA	504	A	C8-N7	7.53	1.36	1.31
22	BA	2740	A	N7-C5	-7.53	1.34	1.39
22	BA	2439	A	C5-C4	-7.53	1.33	1.38
22	BA	2171	A	C8-N7	7.53	1.36	1.31
22	BA	342	A	C5-C4	-7.53	1.33	1.38
22	BA	722	A	C5-C4	-7.52	1.33	1.38
22	BA	1509	A	C8-N7	7.52	1.36	1.31
1	AA	152	A	C8-N7	7.52	1.36	1.31
1	AA	1503	A	C5-C4	-7.51	1.33	1.38
55	B8	51	A	C8-N7	7.51	1.36	1.31
22	BA	2478	A	C5-C4	-7.51	1.33	1.38
1	AA	918	A	C5-C4	-7.51	1.33	1.38
1	AA	573	A	C5-C4	-7.50	1.33	1.38
22	BA	244	A	C5-C4	-7.50	1.33	1.38
1	AA	907	A	C5-C4	-7.50	1.33	1.38
22	BA	2430	A	N7-C5	-7.50	1.34	1.39
22	BA	160	A	C5-C4	-7.49	1.33	1.38
22	BA	1080	A	C8-N7	7.49	1.36	1.31
1	AA	309	A	C5-C4	-7.48	1.33	1.38
1	AA	878	A	C5-C4	-7.48	1.33	1.38
22	BA	443	A	C5-C4	-7.47	1.33	1.38
22	BA	218	A	C5-C4	-7.47	1.33	1.38
22	BA	2173	A	C8-N7	7.47	1.36	1.31
1	AA	1441	A	C8-N7	7.47	1.36	1.31
1	AA	1000	A	C8-N7	7.46	1.36	1.31
22	BA	300	A	C5-C4	-7.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2809	A	C5-C4	-7.46	1.33	1.38
1	AA	336	A	C5-C4	-7.46	1.33	1.38
22	BA	1580	A	C5-C4	-7.46	1.33	1.38
22	BA	470	A	C5-C4	-7.46	1.33	1.38
22	BA	1307	A	C5-C4	-7.46	1.33	1.38
1	AA	807	A	C5-C4	-7.45	1.33	1.38
22	BA	1496	A	C5-C4	-7.45	1.33	1.38
22	BA	2736	A	C5-C4	-7.45	1.33	1.38
22	BA	21	A	C5-C4	-7.45	1.33	1.38
22	BA	173	A	C5-C4	-7.45	1.33	1.38
22	BA	1040	A	C5-C4	-7.45	1.33	1.38
22	BA	144	A	C5-C4	-7.45	1.33	1.38
1	AA	236	A	C5-C4	-7.44	1.33	1.38
1	AA	1179	A	C8-N7	7.44	1.36	1.31
22	BA	2705	A	C5-C4	-7.44	1.33	1.38
1	AA	1035	A	C8-N7	7.44	1.36	1.31
22	BA	346	A	C5-C4	-7.43	1.33	1.38
22	BA	2602	A	C8-N7	7.43	1.36	1.31
1	AA	815	A	C5-C4	-7.43	1.33	1.38
1	AA	1534	A	C8-N7	7.43	1.36	1.31
1	AA	1155	A	C8-N7	7.43	1.36	1.31
23	BB	29	A	C5-C4	-7.43	1.33	1.38
55	B8	38	A	C8-N7	7.43	1.36	1.31
1	AA	78	A	C8-N7	7.41	1.36	1.31
1	AA	539	A	C5-C4	-7.41	1.33	1.38
22	BA	1858	A	C5-C4	-7.41	1.33	1.38
22	BA	2154	A	C8-N7	7.41	1.36	1.31
55	B8	6	A	C8-N7	7.41	1.36	1.31
1	AA	767	A	C5-C4	-7.41	1.33	1.38
22	BA	1027	A	C5-C4	-7.41	1.33	1.38
22	BA	1809	A	N7-C5	-7.40	1.34	1.39
22	BA	1678	A	N7-C5	-7.40	1.34	1.39
1	AA	1508	A	C5-C4	-7.40	1.33	1.38
22	BA	429	A	C5-C4	-7.40	1.33	1.38
22	BA	721	A	C5-C4	-7.40	1.33	1.38
22	BA	655	A	C5-C4	-7.39	1.33	1.38
22	BA	2432	A	C5-C4	-7.39	1.33	1.38
55	B8	26	A	C8-N7	7.39	1.36	1.31
1	AA	282	A	C5-C4	-7.39	1.33	1.38
1	AA	906	A	C5-C4	-7.39	1.33	1.38
22	BA	2311	A	C8-N7	7.39	1.36	1.31
22	BA	2388	A	N9-C8	-7.39	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1598	A	C5-C4	-7.38	1.33	1.38
22	BA	2882	A	C5-C4	-7.38	1.33	1.38
1	AA	1418	A	C5-C4	-7.37	1.33	1.38
22	BA	1069	A	C8-N7	7.37	1.36	1.31
22	BA	1085	A	C8-N7	7.37	1.36	1.31
1	AA	1465	A	C5-C4	-7.37	1.33	1.38
22	BA	556	A	C5-C4	-7.37	1.33	1.38
22	BA	1304	A	C5-C4	-7.37	1.33	1.38
22	BA	1528	A	C5-C4	-7.37	1.33	1.38
22	BA	181	A	C8-N7	7.36	1.36	1.31
22	BA	983	A	N7-C5	-7.36	1.34	1.39
22	BA	2108	A	C8-N7	7.36	1.36	1.31
22	BA	1877	A	C5-C4	-7.36	1.33	1.38
1	AA	461	A	C8-N7	7.36	1.36	1.31
1	AA	412	A	C8-N7	7.35	1.36	1.31
22	BA	2879	A	C5-C4	-7.35	1.33	1.38
22	BA	167	A	C5-C4	-7.35	1.33	1.38
22	BA	1918	A	C5-C4	-7.35	1.33	1.38
22	BA	2587	A	C5-C4	-7.34	1.33	1.38
1	AA	26	A	C5-C4	-7.34	1.33	1.38
23	BB	50	A	C5-C4	-7.33	1.33	1.38
22	BA	374	A	C5-C4	-7.33	1.33	1.38
23	BB	34	A	C5-C4	-7.33	1.33	1.38
23	BB	101	A	C5-C4	-7.33	1.33	1.38
22	BA	2198	A	C5-C4	-7.33	1.33	1.38
1	AA	498	A	C5-C4	-7.32	1.33	1.38
1	AA	313	A	C5-C4	-7.32	1.33	1.38
1	AA	825	A	C5-C4	-7.32	1.33	1.38
22	BA	265	A	C5-C4	-7.32	1.33	1.38
22	BA	925	A	C5-C4	-7.32	1.33	1.38
22	BA	2134	A	C8-N7	7.32	1.36	1.31
1	AA	694	A	C5-C4	-7.31	1.33	1.38
22	BA	2126	A	C8-N7	7.31	1.36	1.31
22	BA	2322	A	C5-C4	-7.31	1.33	1.38
22	BA	1088	A	C8-N7	7.30	1.36	1.31
1	AA	1319	A	C8-N7	7.30	1.36	1.31
1	AA	1468	A	C5-C4	-7.30	1.33	1.38
22	BA	1603	A	C5-C4	-7.30	1.33	1.38
22	BA	2566	A	C5-C4	-7.30	1.33	1.38
22	BA	522	A	N7-C5	-7.30	1.34	1.39
1	AA	1377	A	C8-N7	7.30	1.36	1.31
22	BA	1713	A	C5-C4	-7.29	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2095	A	C5-C4	-7.29	1.33	1.38
22	BA	1854	A	N7-C5	-7.29	1.34	1.39
22	BA	391	A	C5-C4	-7.29	1.33	1.38
22	BA	1593	A	C5-C4	-7.29	1.33	1.38
55	B8	21	A	C8-N7	7.29	1.36	1.31
1	AA	768	A	C5-C4	-7.28	1.33	1.38
22	BA	2721	A	N7-C5	-7.28	1.34	1.39
22	BA	2117	A	C8-N7	7.28	1.36	1.31
1	AA	179	A	C8-N7	7.28	1.36	1.31
1	AA	996	A	C8-N7	7.28	1.36	1.31
22	BA	1477	A	C5-C4	-7.28	1.33	1.38
22	BA	2377	A	C5-C4	-7.28	1.33	1.38
22	BA	1676	A	C5-C4	-7.28	1.33	1.38
55	B8	58	A	C8-N7	7.27	1.36	1.31
1	AA	937	A	C5-C4	-7.27	1.33	1.38
22	BA	2453	A	N7-C5	-7.27	1.34	1.39
1	AA	596	A	C5-C4	-7.27	1.33	1.38
22	BA	103	A	C5-C4	-7.27	1.33	1.38
22	BA	1544	A	C5-C4	-7.27	1.33	1.38
22	BA	1757	A	C5-C4	-7.27	1.33	1.38
22	BA	299	A	C5-C4	-7.26	1.33	1.38
1	AA	303	A	C5-C4	-7.26	1.33	1.38
1	AA	892	A	C5-C4	-7.26	1.33	1.38
1	AA	914	A	C5-C4	-7.26	1.33	1.38
22	BA	1077	A	C8-N7	7.26	1.36	1.31
1	AA	363	A	C5-C4	-7.26	1.33	1.38
1	AA	1480	A	C5-C4	-7.26	1.33	1.38
22	BA	344	A	C5-C4	-7.26	1.33	1.38
22	BA	1866	A	C5-C4	-7.26	1.33	1.38
22	BA	1785	A	C5-C4	-7.26	1.33	1.38
1	AA	1105	A	C8-N7	7.25	1.36	1.31
55	B8	42	A	C8-N7	7.25	1.36	1.31
1	AA	28	A	C5-C4	-7.25	1.33	1.38
22	BA	572	A	N7-C5	-7.25	1.34	1.39
22	BA	2761	A	C5-C4	-7.25	1.33	1.38
1	AA	143	A	C8-N7	7.25	1.36	1.31
1	AA	466	A	C8-N7	7.25	1.36	1.31
22	BA	282	A	C8-N7	7.24	1.36	1.31
22	BA	1213	A	N7-C5	-7.24	1.34	1.39
22	BA	1420	A	C8-N7	7.24	1.36	1.31
22	BA	1762	A	C5-C4	-7.24	1.33	1.38
22	BA	2407	A	C5-C4	-7.24	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1571	A	N7-C5	-7.24	1.34	1.39
22	BA	492	A	C5-C4	-7.23	1.33	1.38
1	AA	935	A	C5-C4	-7.23	1.33	1.38
22	BA	1039	A	C5-C4	-7.23	1.33	1.38
22	BA	2856	A	C5-C4	-7.23	1.33	1.38
22	BA	2727	A	N7-C5	-7.23	1.34	1.39
22	BA	1264	A	N7-C5	-7.23	1.34	1.39
55	B8	66	A	C8-N7	7.22	1.36	1.31
1	AA	607	A	C8-N7	7.22	1.36	1.31
1	AA	1507	A	C5-C4	-7.22	1.33	1.38
22	BA	1103	A	C8-N7	7.21	1.36	1.31
1	AA	243	A	C5-C4	-7.21	1.33	1.38
1	AA	1016	A	C8-N7	7.21	1.36	1.31
1	AA	1398	A	C5-C4	-7.21	1.33	1.38
22	BA	2184	A	C8-N7	7.21	1.36	1.31
1	AA	1130	A	C8-N7	7.21	1.36	1.31
1	AA	1157	A	C8-N7	7.21	1.36	1.31
22	BA	1503	A	C5-C4	-7.21	1.33	1.38
22	BA	161	A	C5-C4	-7.20	1.33	1.38
22	BA	547	A	N3-C4	7.20	1.39	1.34
22	BA	1089	A	C8-N7	7.20	1.36	1.31
22	BA	401	A	N7-C5	-7.20	1.34	1.39
22	BA	896	A	C8-N7	7.20	1.36	1.31
1	AA	371	A	C5-C4	-7.20	1.33	1.38
1	AA	1044	A	C8-N7	7.20	1.36	1.31
1	AA	3	A	C8-N7	7.19	1.36	1.31
1	AA	196	A	C8-N7	7.19	1.36	1.31
1	AA	315	A	C5-C4	-7.19	1.33	1.38
1	AA	648	A	C8-N7	7.19	1.36	1.31
54	B7	9	A	C8-N7	7.19	1.36	1.31
22	BA	2366	A	C5-C4	-7.19	1.33	1.38
22	BA	2753	A	C5-C4	-7.19	1.33	1.38
22	BA	1321	A	C8-N7	7.18	1.36	1.31
22	BA	1241	A	C5-C4	-7.18	1.33	1.38
22	BA	354	A	C8-N7	7.18	1.36	1.31
22	BA	1532	A	C8-N7	7.18	1.36	1.31
22	BA	2020	A	N7-C5	-7.18	1.34	1.39
22	BA	892	A	C8-N7	7.17	1.36	1.31
22	BA	2163	A	N3-C4	7.17	1.39	1.34
22	BA	820	A	N7-C5	-7.17	1.34	1.39
22	BA	1434	A	C5-C4	-7.17	1.33	1.38
22	BA	1705	A	C5-C4	-7.17	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2530	A	C5-C4	-7.17	1.33	1.38
1	AA	546	A	C5-C4	-7.17	1.33	1.38
1	AA	873	A	C5-C4	-7.17	1.33	1.38
22	BA	1046	A	C8-N7	7.16	1.36	1.31
22	BA	1175	A	N3-C4	7.16	1.39	1.34
1	AA	574	A	C5-C4	-7.15	1.33	1.38
1	AA	790	A	C5-C4	-7.15	1.33	1.38
22	BA	1504	A	C5-C4	-7.15	1.33	1.38
1	AA	622	A	C8-N7	7.15	1.36	1.31
22	BA	866	A	C5-C4	-7.15	1.33	1.38
1	AA	704	A	C5-C4	-7.15	1.33	1.38
22	BA	1322	A	C5-C4	-7.15	1.33	1.38
22	BA	241	A	C5-C4	-7.14	1.33	1.38
1	AA	460	A	C8-N7	7.14	1.36	1.31
22	BA	1938	A	C5-C4	-7.14	1.33	1.38
1	AA	155	A	C8-N7	7.14	1.36	1.31
1	AA	532	A	C8-N7	7.13	1.36	1.31
1	AA	716	A	C5-C4	-7.13	1.33	1.38
1	AA	978	A	C8-N7	7.13	1.36	1.31
22	BA	1640	A	C5-C4	-7.13	1.33	1.38
1	AA	958	A	C8-N7	7.12	1.36	1.31
22	BA	981	A	N7-C5	-7.12	1.34	1.39
1	AA	676	A	C5-C4	-7.11	1.33	1.38
1	AA	600	A	C5-C4	-7.10	1.33	1.38
22	BA	1515	A	C5-C4	-7.10	1.33	1.38
22	BA	528	A	C5-C4	-7.10	1.33	1.38
23	BB	53	A	C5-C4	-7.09	1.33	1.38
1	AA	189	A	C8-N7	7.09	1.36	1.31
22	BA	480	A	C5-C4	-7.09	1.33	1.38
1	AA	465	A	C8-N7	7.08	1.36	1.31
22	BA	182	A	C5-C4	-7.08	1.33	1.38
22	BA	2868	A	C5-C4	-7.08	1.33	1.38
1	AA	510	A	C5-C4	-7.08	1.33	1.38
1	AA	909	A	C5-C4	-7.08	1.33	1.38
22	BA	1067	A	C8-N7	7.08	1.36	1.31
22	BA	2309	A	C8-N7	7.08	1.36	1.31
1	AA	1080	A	C5-C4	-7.07	1.33	1.38
1	AA	1257	A	C8-N7	7.07	1.36	1.31
1	AA	1012	A	C8-N7	7.06	1.36	1.31
22	BA	849	A	C5-C4	-7.06	1.33	1.38
1	AA	1092	A	C8-N7	7.06	1.36	1.31
22	BA	2147	A	C8-N7	7.06	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2634	A	C5-C4	-7.06	1.33	1.38
22	BA	1583	A	C8-N7	7.05	1.36	1.31
1	AA	250	A	C8-N7	7.05	1.36	1.31
22	BA	793	A	C5-C4	-7.05	1.33	1.38
1	AA	253	A	C5-C4	-7.04	1.33	1.38
1	AA	338	A	C5-C4	-7.04	1.33	1.38
1	AA	1081	A	C5-C4	-7.04	1.33	1.38
22	BA	2297	A	C5-C4	-7.04	1.33	1.38
22	BA	1098	A	C8-N7	7.04	1.36	1.31
55	B8	14	A	C8-N7	7.04	1.36	1.31
22	BA	2577	A	N7-C5	-7.04	1.35	1.39
1	AA	2	A	C8-N7	7.03	1.36	1.31
1	AA	60	A	C5-C4	-7.03	1.33	1.38
1	AA	1346	A	C5-C4	-7.03	1.33	1.38
22	BA	2813	A	C5-C4	-7.03	1.33	1.38
22	BA	190	A	N7-C5	-7.03	1.35	1.39
22	BA	322	A	C5-C4	-7.02	1.33	1.38
1	AA	228	A	C5-C4	-7.02	1.33	1.38
22	BA	750	A	N7-C5	-7.02	1.35	1.39
1	AA	431	A	C8-N7	7.02	1.36	1.31
22	BA	270	A	C5-C4	-7.01	1.33	1.38
22	BA	1000	A	N7-C5	-7.01	1.35	1.39
55	B8	69	A	C8-N7	7.01	1.36	1.31
22	BA	1654	A	C5-C4	-7.01	1.33	1.38
1	AA	696	A	C5-C4	-7.00	1.33	1.38
1	AA	553	A	C5-C4	-7.00	1.33	1.38
22	BA	603	A	C5-C4	-7.00	1.33	1.38
1	AA	495	A	C8-N7	7.00	1.36	1.31
22	BA	1745	A	C5-C4	-7.00	1.33	1.38
1	AA	80	A	N3-C4	6.99	1.39	1.34
1	AA	120	A	C5-C4	-6.99	1.33	1.38
1	AA	192	A	C8-N7	6.99	1.36	1.31
1	AA	195	A	C8-N7	6.99	1.36	1.31
22	BA	1057	A	C8-N7	6.99	1.36	1.31
1	AA	1035	A	N3-C4	6.99	1.39	1.34
22	BA	972	A	N7-C5	-6.98	1.35	1.39
1	AA	1288	A	C8-N7	6.98	1.36	1.31
1	AA	1261	A	C8-N7	6.98	1.36	1.31
1	AA	969	A	C5-C4	-6.97	1.33	1.38
22	BA	2346	A	C5-C4	-6.97	1.33	1.38
1	AA	1396	A	C5-C4	-6.97	1.33	1.38
22	BA	2211	A	C8-N7	6.97	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2835	A	C5-C4	-6.97	1.33	1.38
1	AA	119	A	C8-N7	6.97	1.36	1.31
22	BA	2564	A	N7-C5	-6.96	1.35	1.39
1	AA	451	A	C8-N7	6.96	1.36	1.31
22	BA	255	A	C5-C4	-6.96	1.33	1.38
22	BA	1773	A	N7-C5	-6.96	1.35	1.39
1	AA	1105	A	C5-C4	-6.96	1.33	1.38
1	AA	1019	A	C8-N7	6.96	1.36	1.31
22	BA	1503	A	C8-N7	6.96	1.36	1.31
22	BA	878	A	C8-N7	6.96	1.36	1.31
1	AA	389	A	C5-C4	-6.95	1.33	1.38
1	AA	1167	A	C8-N7	6.95	1.36	1.31
22	BA	513	A	N7-C5	-6.95	1.35	1.39
1	AA	729	A	C5-C4	-6.95	1.33	1.38
22	BA	1134	A	C5-C4	-6.95	1.33	1.38
1	AA	1163	A	C8-N7	6.95	1.36	1.31
1	AA	1410	A	C5-C4	-6.95	1.33	1.38
22	BA	877	A	C8-N7	6.95	1.36	1.31
1	AA	51	A	C5-C4	-6.95	1.33	1.38
1	AA	1492	A	C8-N7	6.95	1.36	1.31
22	BA	1504	A	C8-N7	6.95	1.36	1.31
1	AA	642	A	C5-C4	-6.94	1.33	1.38
1	AA	1269	A	C8-N7	6.94	1.36	1.31
22	BA	2135	A	N3-C4	6.94	1.39	1.34
22	BA	2169	A	C8-N7	6.94	1.36	1.31
1	AA	496	A	C8-N7	6.94	1.36	1.31
1	AA	535	A	C5-C4	-6.94	1.33	1.38
22	BA	44	A	C5-C4	-6.94	1.33	1.38
1	AA	1229	A	C5-C4	-6.94	1.33	1.38
22	BA	1070	A	C8-N7	6.93	1.36	1.31
1	AA	563	A	C5-C4	-6.93	1.33	1.38
1	AA	1176	A	C8-N7	6.93	1.36	1.31
22	BA	2117	A	N3-C4	6.93	1.39	1.34
22	BA	1354	A	N7-C5	-6.93	1.35	1.39
22	BA	1354	A	N9-C8	-6.93	1.32	1.37
55	B8	41	A	C8-N7	6.92	1.36	1.31
1	AA	78	A	N3-C4	6.92	1.39	1.34
22	BA	2158	A	N3-C4	6.92	1.39	1.34
22	BA	1111	A	C5-C4	-6.92	1.33	1.38
22	BA	1495	A	C5-C4	-6.92	1.33	1.38
1	AA	747	A	C8-N7	6.92	1.36	1.31
1	AA	908	A	C5-C4	-6.91	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	695	A	C5-C4	-6.91	1.33	1.38
22	BA	2241	A	N7-C5	-6.91	1.35	1.39
22	BA	793	A	N7-C5	-6.91	1.35	1.39
22	BA	1912	A	C5-C4	-6.90	1.33	1.38
22	BA	172	A	C5-C4	-6.90	1.33	1.38
22	BA	368	A	C5-C4	-6.90	1.33	1.38
55	B8	59	A	C8-N7	6.90	1.36	1.31
22	BA	1635	A	C5-C4	-6.90	1.33	1.38
22	BA	63	A	C5-C4	-6.89	1.33	1.38
22	BA	905	A	C5-C4	-6.89	1.33	1.38
1	AA	33	A	C5-C4	-6.89	1.33	1.38
1	AA	923	A	C5-C4	-6.89	1.33	1.38
1	AA	1437	A	C5-C4	-6.89	1.33	1.38
22	BA	1143	A	N7-C5	-6.89	1.35	1.39
1	AA	205	A	C8-N7	6.88	1.36	1.31
22	BA	1586	A	C8-N7	6.88	1.36	1.31
22	BA	505	A	C5-C4	-6.88	1.33	1.38
1	AA	1	A	C8-N7	6.88	1.36	1.31
1	AA	238	A	C5-C4	-6.88	1.33	1.38
1	AA	1285	A	C8-N7	6.88	1.36	1.31
1	AA	1311	A	C5-C4	-6.88	1.33	1.38
1	AA	728	A	C5-C4	-6.88	1.33	1.38
22	BA	705	A	N7-C5	-6.88	1.35	1.39
1	AA	274	A	C8-N7	6.87	1.36	1.31
1	AA	298	A	C5-C4	-6.87	1.33	1.38
1	AA	1274	A	C8-N7	6.87	1.36	1.31
1	AA	411	A	C5-C4	-6.87	1.33	1.38
22	BA	1383	A	C5-C4	-6.87	1.33	1.38
22	BA	2705	A	N7-C5	-6.87	1.35	1.39
22	BA	2430	A	C5-C4	-6.87	1.33	1.38
1	AA	609	A	C5-C4	-6.86	1.33	1.38
1	AA	889	A	C5-C4	-6.86	1.33	1.38
22	BA	1050	A	C8-N7	6.86	1.36	1.31
22	BA	2900	A	C8-N7	6.86	1.36	1.31
1	AA	946	A	C5-C4	-6.86	1.33	1.38
1	AA	1236	A	C5-C4	-6.86	1.33	1.38
23	BB	34	A	C8-N7	6.85	1.36	1.31
1	AA	743	A	C5-C4	-6.85	1.33	1.38
1	AA	435	A	C8-N7	6.85	1.36	1.31
1	AA	663	A	C5-C4	-6.85	1.33	1.38
1	AA	831	A	C5-C4	-6.85	1.33	1.38
22	BA	1096	A	N3-C4	6.85	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	933	A	C5-C4	-6.85	1.33	1.38
1	AA	181	A	C8-N7	6.85	1.36	1.31
1	AA	263	A	C5-C4	-6.85	1.33	1.38
22	BA	2101	A	C8-N7	6.84	1.36	1.31
1	AA	162	A	C5-C4	-6.84	1.33	1.38
1	AA	246	A	C5-C4	-6.84	1.33	1.38
1	AA	819	A	C5-C4	-6.84	1.33	1.38
22	BA	2800	A	C8-N7	6.84	1.36	1.31
1	AA	373	A	C5-C4	-6.84	1.33	1.38
1	AA	872	A	C5-C4	-6.84	1.33	1.38
1	AA	1101	A	C5-C4	-6.84	1.33	1.38
22	BA	2719	G	C8-N7	-6.84	1.26	1.30
1	AA	329	A	C5-C4	-6.84	1.33	1.38
1	AA	8	A	C5-C4	-6.84	1.33	1.38
1	AA	949	A	C5-C4	-6.83	1.33	1.38
1	AA	1329	A	C8-N7	6.83	1.36	1.31
1	AA	608	A	C5-C4	-6.83	1.33	1.38
1	AA	1362	A	C5-C4	-6.83	1.33	1.38
22	BA	1084	A	C8-N7	6.83	1.36	1.31
22	BA	155	A	C5-C4	-6.83	1.33	1.38
22	BA	156	A	C5-C4	-6.82	1.33	1.38
22	BA	1502	A	C5-C4	-6.82	1.33	1.38
22	BA	149	A	C5-C4	-6.82	1.33	1.38
22	BA	352	A	C8-N7	6.82	1.36	1.31
22	BA	2614	A	N7-C5	-6.82	1.35	1.39
1	AA	182	A	C5-C4	-6.82	1.33	1.38
22	BA	654	A	N3-C4	6.82	1.39	1.34
22	BA	1090	A	N3-C4	6.82	1.39	1.34
22	BA	415	A	N7-C5	-6.82	1.35	1.39
1	AA	50	A	C5-C4	-6.82	1.33	1.38
22	BA	1746	A	C5-C4	-6.82	1.33	1.38
22	BA	384	A	N7-C5	-6.81	1.35	1.39
22	BA	404	A	C5-C4	-6.81	1.33	1.38
1	AA	1005	A	C8-N7	6.81	1.36	1.31
1	AA	1101	A	C8-N7	6.81	1.36	1.31
1	AA	1246	A	C8-N7	6.81	1.36	1.31
22	BA	1616	A	N7-C5	-6.81	1.35	1.39
22	BA	1490	A	C8-N7	6.80	1.36	1.31
22	BA	1111	A	C8-N7	6.80	1.36	1.31
1	AA	44	A	C8-N7	6.80	1.36	1.31
1	AA	1152	A	C8-N7	6.80	1.36	1.31
1	AA	131	A	C5-C4	-6.80	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	71	A	C5-C4	-6.80	1.33	1.38
22	BA	829	A	C5-C4	-6.80	1.33	1.38
1	AA	1289	A	C8-N7	6.79	1.36	1.31
1	AA	1251	A	C8-N7	6.79	1.36	1.31
22	BA	1254	A	N7-C5	-6.79	1.35	1.39
1	AA	282	A	C8-N7	6.78	1.36	1.31
22	BA	1569	A	N7-C5	-6.78	1.35	1.39
22	BA	1419	A	C8-N7	6.78	1.36	1.31
22	BA	1669	A	C5-C4	-6.78	1.34	1.38
22	BA	2082	A	N7-C5	-6.78	1.35	1.39
1	AA	1204	A	C8-N7	6.78	1.36	1.31
1	AA	139	A	C8-N7	6.78	1.36	1.31
1	AA	502	A	C5-C4	-6.78	1.34	1.38
1	AA	1434	A	C5-C4	-6.77	1.34	1.38
1	AA	1004	A	C8-N7	6.77	1.36	1.31
1	AA	1299	A	C8-N7	6.77	1.36	1.31
22	BA	675	A	N7-C5	-6.77	1.35	1.39
23	BB	73	A	C5-C4	-6.77	1.34	1.38
1	AA	7	A	C5-C4	-6.77	1.34	1.38
1	AA	243	A	C8-N7	6.77	1.36	1.31
1	AA	621	A	C8-N7	6.77	1.36	1.31
1	AA	1042	A	N3-C4	6.77	1.39	1.34
22	BA	2077	A	N7-C5	-6.77	1.35	1.39
22	BA	2378	A	C5-C4	-6.77	1.34	1.38
22	BA	2820	A	C5-C4	-6.76	1.34	1.38
1	AA	520	A	C8-N7	6.76	1.36	1.31
22	BA	616	A	C5-C4	-6.76	1.34	1.38
1	AA	72	A	C8-N7	6.76	1.36	1.31
22	BA	614	A	C8-N7	6.76	1.36	1.31
22	BA	2070	A	N7-C5	-6.76	1.35	1.39
1	AA	1332	A	C8-N7	6.75	1.36	1.31
1	AA	393	A	C5-C4	-6.75	1.34	1.38
22	BA	1021	A	C5-C4	-6.75	1.34	1.38
22	BA	13	A	N7-C5	-6.75	1.35	1.39
22	BA	2317	A	C5-C4	-6.75	1.34	1.38
1	AA	109	A	C5-C4	-6.75	1.34	1.38
1	AA	1368	A	C5-C4	-6.75	1.34	1.38
22	BA	782	A	N7-C5	-6.75	1.35	1.39
1	AA	753	A	C5-C4	-6.75	1.34	1.38
1	AA	1339	A	C5-C4	-6.75	1.34	1.38
22	BA	2435	A	N9-C8	-6.75	1.32	1.37
1	AA	600	A	C8-N7	6.75	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1735	A	C8-N7	6.75	1.36	1.31
1	AA	306	A	C8-N7	6.74	1.36	1.31
1	AA	1430	A	C5-C4	-6.74	1.34	1.38
22	BA	104	A	C5-C4	-6.74	1.34	1.38
1	AA	622	A	C5-C4	-6.74	1.34	1.38
1	AA	780	A	N7-C5	-6.74	1.35	1.39
22	BA	1780	A	C5-C4	-6.73	1.34	1.38
1	AA	1180	A	C8-N7	6.73	1.36	1.31
22	BA	1789	A	N7-C5	-6.73	1.35	1.39
1	AA	161	A	C5-C4	-6.73	1.34	1.38
22	BA	404	A	C8-N7	6.73	1.36	1.31
22	BA	984	A	N7-C5	-6.73	1.35	1.39
1	AA	171	A	C8-N7	6.73	1.36	1.31
1	AA	1197	A	C5-C4	-6.72	1.34	1.38
22	BA	2126	A	N3-C4	6.72	1.38	1.34
22	BA	2733	A	C5-C4	-6.72	1.34	1.38
22	BA	272	A	C5-C4	-6.72	1.34	1.38
22	BA	1590	A	C8-N7	6.72	1.36	1.31
22	BA	2749	A	C5-C4	-6.72	1.34	1.38
1	AA	130	A	C5-C4	-6.72	1.34	1.38
1	AA	1082	A	C5-C4	-6.72	1.34	1.38
1	AA	1102	A	C5-C4	-6.72	1.34	1.38
1	AA	60	A	C8-N7	6.71	1.36	1.31
1	AA	262	A	C5-C4	-6.71	1.34	1.38
1	AA	864	A	C5-C4	-6.71	1.34	1.38
1	AA	129	A	C8-N7	6.71	1.36	1.31
1	AA	1014	A	C8-N7	6.71	1.36	1.31
1	AA	66	A	C5-C4	-6.71	1.34	1.38
22	BA	1579	A	C5-C4	-6.71	1.34	1.38
1	AA	1280	A	C8-N7	6.71	1.36	1.31
22	BA	2170	A	N3-C4	6.71	1.38	1.34
22	BA	2886	A	C5-C4	-6.71	1.34	1.38
22	BA	2142	A	C8-N7	6.70	1.36	1.31
1	AA	415	A	C8-N7	6.70	1.36	1.31
22	BA	1133	A	N7-C5	-6.70	1.35	1.39
1	AA	938	A	C5-C4	-6.70	1.34	1.38
22	BA	1876	A	C8-N7	6.70	1.36	1.31
22	BA	2542	A	N7-C5	-6.70	1.35	1.39
1	AA	171	A	C5-C4	-6.69	1.34	1.38
22	BA	2592	G	C8-N7	-6.69	1.26	1.30
1	AA	408	A	C8-N7	6.69	1.36	1.31
1	AA	509	A	C5-C4	-6.69	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	547	A	C8-N7	6.69	1.36	1.31
1	AA	1346	A	C8-N7	6.69	1.36	1.31
1	AA	1360	A	C8-N7	6.69	1.36	1.31
22	BA	278	A	C8-N7	6.69	1.36	1.31
22	BA	1810	A	N7-C5	-6.69	1.35	1.39
1	AA	68	G	N9-C4	6.68	1.43	1.38
22	BA	347	A	C5-C4	-6.68	1.34	1.38
1	AA	554	A	C8-N7	6.68	1.36	1.31
1	AA	1329	A	C5-C4	-6.68	1.34	1.38
22	BA	1808	A	C5-C4	-6.68	1.34	1.38
22	BA	2314	A	C5-C4	-6.67	1.34	1.38
22	BA	2850	A	N7-C5	-6.67	1.35	1.39
23	BB	59	A	C5-C4	-6.67	1.34	1.38
1	AA	554	A	C5-C4	-6.67	1.34	1.38
1	AA	1349	A	C5-C4	-6.67	1.34	1.38
1	AA	712	A	C5-C4	-6.67	1.34	1.38
1	AA	1196	A	C8-N7	6.66	1.36	1.31
22	BA	2171	A	N3-C4	6.66	1.38	1.34
22	BA	508	A	C8-N7	6.66	1.36	1.31
1	AA	1067	A	C5-C4	-6.66	1.34	1.38
22	BA	1453	A	C5-C4	-6.66	1.34	1.38
22	BA	699	A	N7-C5	-6.66	1.35	1.39
22	BA	896	A	N3-C4	6.66	1.38	1.34
22	BA	1754	A	N7-C5	-6.66	1.35	1.39
1	AA	246	A	C8-N7	6.65	1.36	1.31
22	BA	608	A	N7-C5	-6.65	1.35	1.39
22	BA	2071	A	N7-C5	-6.65	1.35	1.39
22	BA	2820	A	C8-N7	6.65	1.36	1.31
1	AA	55	A	C8-N7	6.64	1.36	1.31
1	AA	160	A	C5-C4	-6.64	1.34	1.38
22	BA	2800	A	C5-C4	-6.64	1.34	1.38
1	AA	344	A	C8-N7	6.64	1.36	1.31
1	AA	1169	A	C8-N7	6.64	1.36	1.31
1	AA	1357	A	C8-N7	6.64	1.36	1.31
22	BA	920	A	N7-C5	-6.64	1.35	1.39
1	AA	1146	A	C8-N7	6.64	1.36	1.31
22	BA	1226	A	N7-C5	-6.64	1.35	1.39
1	AA	223	A	C8-N7	6.64	1.36	1.31
22	BA	1050	A	C5-C4	-6.64	1.34	1.38
1	AA	50	A	C8-N7	6.64	1.36	1.31
22	BA	2114	A	C8-N7	6.64	1.36	1.31
1	AA	1271	A	C8-N7	6.63	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2176	A	C8-N7	6.63	1.36	1.31
22	BA	91	A	C5-C4	-6.63	1.34	1.38
22	BA	2406	A	C5-C4	-6.63	1.34	1.38
22	BA	574	A	N7-C5	-6.63	1.35	1.39
1	AA	459	A	C8-N7	6.63	1.36	1.31
1	AA	964	A	C5-C4	-6.62	1.34	1.38
22	BA	1205	A	C5-C4	-6.62	1.34	1.38
1	AA	520	A	C5-C4	-6.62	1.34	1.38
1	AA	602	A	C5-C4	-6.62	1.34	1.38
1	AA	1311	A	C8-N7	6.62	1.36	1.31
23	BB	52	A	C5-C4	-6.62	1.34	1.38
22	BA	1853	A	N7-C5	-6.62	1.35	1.39
1	AA	1216	A	C8-N7	6.62	1.36	1.31
1	AA	448	A	C8-N7	6.62	1.36	1.31
1	AA	1446	A	C8-N7	6.62	1.36	1.31
1	AA	101	A	C8-N7	6.61	1.36	1.31
22	BA	900	A	C8-N7	6.61	1.36	1.31
1	AA	2	A	C5-C4	-6.61	1.34	1.38
1	AA	1340	A	C5-C4	-6.61	1.34	1.38
1	AA	53	A	C5-C4	-6.61	1.34	1.38
1	AA	80	A	C8-N7	6.61	1.36	1.31
22	BA	142	A	C8-N7	6.61	1.36	1.31
22	BA	146	A	C5-C4	-6.61	1.34	1.38
22	BA	980	A	N7-C5	-6.61	1.35	1.39
1	AA	32	A	C5-C4	-6.61	1.34	1.38
1	AA	1239	A	C8-N7	6.61	1.36	1.31
22	BA	95	A	C5-C4	-6.60	1.34	1.38
22	BA	1871	A	C8-N7	6.60	1.36	1.31
22	BA	2560	A	N7-C5	-6.60	1.35	1.39
22	BA	2298	A	C5-C4	-6.60	1.34	1.38
1	AA	374	A	C5-C4	-6.60	1.34	1.38
1	AA	482	A	C5-C4	-6.60	1.34	1.38
22	BA	718	A	C5-C4	-6.60	1.34	1.38
22	BA	526	A	N7-C5	-6.60	1.35	1.39
1	AA	253	A	C8-N7	6.59	1.36	1.31
22	BA	626	A	C5-C4	-6.59	1.34	1.38
22	BA	2051	A	N7-C5	-6.59	1.35	1.39
1	AA	167	A	C5-C4	-6.59	1.34	1.38
1	AA	441	A	C5-C4	-6.59	1.34	1.38
1	AA	149	A	C8-N7	6.58	1.36	1.31
22	BA	899	A	C8-N7	6.58	1.36	1.31
1	AA	81	A	N3-C4	6.58	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	382	A	C8-N7	6.58	1.36	1.31
1	AA	1150	A	C8-N7	6.58	1.36	1.31
22	BA	2015	A	N7-C5	-6.58	1.35	1.39
1	AA	77	A	N3-C4	6.58	1.38	1.34
22	BA	2142	A	N3-C4	6.57	1.38	1.34
22	BA	2169	A	N3-C4	6.57	1.38	1.34
1	AA	1238	A	C8-N7	6.57	1.36	1.31
22	BA	582	A	N7-C5	-6.57	1.35	1.39
1	AA	1254	A	C8-N7	6.57	1.36	1.31
22	BA	2037	A	N7-C5	-6.57	1.35	1.39
1	AA	172	A	C8-N7	6.57	1.36	1.31
1	AA	1248	A	C8-N7	6.57	1.36	1.31
1	AA	7	A	C8-N7	6.56	1.36	1.31
1	AA	983	A	C5-C4	-6.56	1.34	1.38
1	AA	1151	A	N3-C4	6.56	1.38	1.34
1	AA	704	A	C8-N7	6.56	1.36	1.31
22	BA	466	A	N7-C5	-6.56	1.35	1.39
22	BA	1269	A	N7-C5	-6.56	1.35	1.39
22	BA	945	A	N7-C5	-6.56	1.35	1.39
1	AA	1005	A	N3-C4	6.55	1.38	1.34
22	BA	2679	A	N7-C5	-6.55	1.35	1.39
1	AA	1447	A	C8-N7	6.55	1.36	1.31
1	AA	547	A	C5-C4	-6.55	1.34	1.38
22	BA	2061	G	C8-N7	-6.55	1.27	1.30
22	BA	1953	A	N7-C5	-6.55	1.35	1.39
22	BA	1089	A	N3-C4	6.55	1.38	1.34
22	BA	1169	A	C5-C4	-6.55	1.34	1.38
1	AA	1151	A	C8-N7	6.54	1.36	1.31
1	AA	68	G	N9-C8	-6.54	1.33	1.37
22	BA	422	A	N7-C5	-6.54	1.35	1.39
22	BA	1342	A	N7-C5	-6.54	1.35	1.39
1	AA	1256	A	C8-N7	6.54	1.36	1.31
22	BA	1054	A	C8-N7	6.54	1.36	1.31
1	AA	199	A	C8-N7	6.54	1.36	1.31
22	BA	1608	A	N9-C8	-6.54	1.32	1.37
22	BA	2080	A	N7-C5	-6.54	1.35	1.39
22	BA	614	A	C5-C4	-6.54	1.34	1.38
22	BA	472	A	C5-C4	-6.53	1.34	1.38
22	BA	272	A	C8-N7	6.53	1.36	1.31
1	AA	456	A	C8-N7	6.53	1.36	1.31
22	BA	2757	A	C5-C4	-6.53	1.34	1.38
22	BA	1916	A	C5-C4	-6.53	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2900	A	C5-C4	-6.53	1.34	1.38
1	AA	499	A	C8-N7	6.53	1.36	1.31
1	AA	845	A	N3-C4	6.53	1.38	1.34
1	AA	974	A	C5-C4	-6.53	1.34	1.38
1	AA	366	A	C8-N7	6.52	1.36	1.31
1	AA	1251	A	C5-C4	-6.52	1.34	1.38
1	AA	174	A	C8-N7	6.52	1.36	1.31
22	BA	1508	A	C5-C4	-6.52	1.34	1.38
22	BA	1936	A	N7-C5	-6.52	1.35	1.39
1	AA	1110	A	C5-C4	-6.52	1.34	1.38
1	AA	131	A	C8-N7	6.51	1.36	1.31
22	BA	1591	A	C5-C4	-6.51	1.34	1.38
1	AA	270	A	C5-C4	-6.51	1.34	1.38
22	BA	1791	A	N7-C5	-6.51	1.35	1.39
22	BA	1254	A	N9-C8	-6.51	1.32	1.37
22	BA	2837	A	N7-C5	-6.51	1.35	1.39
1	AA	655	A	C8-N7	6.50	1.36	1.31
1	AA	749	A	C8-N7	6.50	1.36	1.31
22	BA	1230	A	C5-C4	-6.50	1.34	1.38
1	AA	994	A	C5-C4	-6.50	1.34	1.38
22	BA	1490	A	N3-C4	6.49	1.38	1.34
1	AA	673	A	C5-C4	-6.49	1.34	1.38
1	AA	499	A	C5-C4	-6.49	1.34	1.38
1	AA	959	A	C5-C4	-6.49	1.34	1.38
1	AA	1377	A	C5-C4	-6.49	1.34	1.38
22	BA	2097	A	C8-N7	6.49	1.36	1.31
1	AA	197	A	C8-N7	6.49	1.36	1.31
22	BA	347	A	C8-N7	6.48	1.36	1.31
22	BA	654	A	C8-N7	6.48	1.36	1.31
22	BA	2273	A	N9-C8	-6.48	1.32	1.37
22	BA	2660	A	C8-N7	6.48	1.36	1.31
1	AA	349	A	C8-N7	6.48	1.36	1.31
22	BA	125	A	C8-N7	6.48	1.36	1.31
1	AA	414	A	C8-N7	6.48	1.36	1.31
22	BA	1677	A	N7-C5	-6.48	1.35	1.39
1	AA	640	A	C8-N7	6.48	1.36	1.31
1	AA	889	A	C8-N7	6.47	1.36	1.31
1	AA	974	A	C8-N7	6.47	1.36	1.31
1	AA	274	A	C5-C4	-6.47	1.34	1.38
53	B5	24	PRO	N-CA	-6.47	1.36	1.47
22	BA	2108	A	N3-C4	6.47	1.38	1.34
22	BA	2686	G	C6-N1	-6.47	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	8	A	C8-N7	6.46	1.36	1.31
1	AA	649	A	C8-N7	6.46	1.36	1.31
1	AA	681	A	C8-N7	6.46	1.36	1.31
22	BA	1899	A	N7-C5	-6.46	1.35	1.39
22	BA	2542	A	N9-C8	-6.46	1.32	1.37
22	BA	752	A	C8-N7	6.46	1.36	1.31
22	BA	1420	A	N3-C4	6.46	1.38	1.34
22	BA	504	A	N3-C4	6.46	1.38	1.34
1	AA	1110	A	C8-N7	6.45	1.36	1.31
1	AA	1250	A	C8-N7	6.45	1.36	1.31
22	BA	2598	A	N7-C5	-6.45	1.35	1.39
1	AA	1287	A	C8-N7	6.45	1.36	1.31
1	AA	1340	A	C8-N7	6.45	1.36	1.31
22	BA	1268	A	N7-C5	-6.45	1.35	1.39
22	BA	1010	A	N7-C5	-6.45	1.35	1.39
22	BA	1590	A	C5-C4	-6.45	1.34	1.38
1	AA	26	A	C8-N7	6.45	1.36	1.31
1	AA	33	A	C8-N7	6.45	1.36	1.31
22	BA	362	A	C8-N7	6.45	1.36	1.31
22	BA	1266	G	C5-C4	-6.45	1.33	1.38
23	BB	15	A	C5-C4	-6.45	1.34	1.38
1	AA	523	A	C5-C4	-6.44	1.34	1.38
22	BA	279	A	C8-N7	6.44	1.36	1.31
22	BA	1069	A	N3-C4	6.44	1.38	1.34
23	BB	57	A	C5-C4	-6.44	1.34	1.38
22	BA	2722	G	C6-N1	-6.44	1.35	1.39
1	AA	325	A	C8-N7	6.44	1.36	1.31
1	AA	1534	A	N3-C4	6.44	1.38	1.34
1	AA	533	A	C8-N7	6.44	1.36	1.31
1	AA	935	A	C8-N7	6.43	1.36	1.31
22	BA	685	A	N7-C5	-6.43	1.35	1.39
1	AA	1111	A	C8-N7	6.43	1.36	1.31
22	BA	1570	A	N7-C5	-6.42	1.35	1.39
23	BB	15	A	C8-N7	6.42	1.36	1.31
1	AA	681	A	C5-C4	-6.42	1.34	1.38
1	AA	1306	A	C5-C4	-6.42	1.34	1.38
22	BA	2386	A	N7-C5	-6.42	1.35	1.39
1	AA	1188	A	C8-N7	6.42	1.36	1.31
1	AA	1333	A	C5-C4	-6.42	1.34	1.38
1	AA	539	A	C8-N7	6.41	1.36	1.31
22	BA	1420	A	C5-C4	-6.41	1.34	1.38
22	BA	528	A	N7-C5	-6.41	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1289	A	C5-C4	-6.41	1.34	1.38
1	AA	411	A	C8-N7	6.41	1.36	1.31
1	AA	393	A	C8-N7	6.40	1.36	1.31
22	BA	1453	A	C8-N7	6.40	1.36	1.31
22	BA	507	A	C8-N7	6.40	1.36	1.31
1	AA	195	A	C5-C4	-6.40	1.34	1.38
1	AA	595	A	C8-N7	6.40	1.36	1.31
1	AA	959	A	C8-N7	6.40	1.36	1.31
22	BA	142	A	C5-C4	-6.40	1.34	1.38
22	BA	1722	A	C5-C4	-6.40	1.34	1.38
1	AA	630	A	C5-C4	-6.39	1.34	1.38
1	AA	1360	A	C5-C4	-6.39	1.34	1.38
22	BA	309	A	N7-C5	-6.39	1.35	1.39
22	BA	730	A	N7-C5	-6.39	1.35	1.39
1	AA	65	A	C8-N7	6.39	1.36	1.31
1	AA	493	A	C8-N7	6.39	1.36	1.31
22	BA	1413	A	C8-N7	6.39	1.36	1.31
22	BA	1689	A	N7-C5	-6.39	1.35	1.39
23	BB	46	A	C5-C4	-6.39	1.34	1.38
1	AA	192	A	C5-C4	-6.39	1.34	1.38
22	BA	2500	U	C2-N3	-6.39	1.33	1.37
1	AA	595	A	C5-C4	-6.38	1.34	1.38
1	AA	1167	A	C5-C4	-6.38	1.34	1.38
22	BA	1378	A	N9-C8	-6.38	1.32	1.37
54	B7	9	A	N3-C4	6.38	1.38	1.34
22	BA	2738	A	N7-C5	-6.38	1.35	1.39
1	AA	1306	A	C8-N7	6.38	1.36	1.31
22	BA	2173	A	N3-C4	6.38	1.38	1.34
1	AA	635	A	C5-C4	-6.38	1.34	1.38
1	AA	1046	A	C8-N7	6.38	1.36	1.31
1	AA	197	A	C5-C4	-6.37	1.34	1.38
1	AA	1375	A	C5-C4	-6.37	1.34	1.38
1	AA	120	A	C8-N7	6.37	1.36	1.31
1	AA	753	A	C8-N7	6.37	1.36	1.31
1	AA	977	A	C5-C4	-6.37	1.34	1.38
22	BA	213	A	C8-N7	6.37	1.36	1.31
1	AA	1456	A	C8-N7	6.37	1.36	1.31
22	BA	1175	A	C8-N7	6.37	1.36	1.31
22	BA	715	A	C5-C4	-6.36	1.34	1.38
1	AA	969	A	C8-N7	6.36	1.36	1.31
22	BA	1070	A	N3-C4	6.36	1.38	1.34
1	AA	435	A	C5-C4	-6.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2425	A	N7-C5	-6.36	1.35	1.39
22	BA	348	A	C5-C4	-6.36	1.34	1.38
22	BA	2682	A	N7-C5	-6.36	1.35	1.39
1	AA	1067	A	C8-N7	6.36	1.35	1.31
1	AA	1363	A	C5-C4	-6.36	1.34	1.38
22	BA	892	A	N3-C4	6.36	1.38	1.34
22	BA	892	A	C3'-O3'	-6.35	1.33	1.42
22	BA	1640	A	C8-N7	6.35	1.35	1.31
22	BA	1803	A	N7-C5	-6.35	1.35	1.39
22	BA	345	A	C5-C4	-6.35	1.34	1.38
22	BA	632	A	N7-C5	-6.35	1.35	1.39
1	AA	468	A	C8-N7	6.35	1.35	1.31
1	AA	1318	A	C8-N7	6.35	1.35	1.31
1	AA	1363	A	C8-N7	6.35	1.35	1.31
22	BA	877	A	C5-C4	-6.35	1.34	1.38
22	BA	1155	A	N7-C5	-6.35	1.35	1.39
1	AA	702	A	C5-C4	-6.34	1.34	1.38
1	AA	759	A	C8-N7	6.34	1.35	1.31
22	BA	718	A	C8-N7	6.34	1.35	1.31
22	BA	941	A	N7-C5	-6.34	1.35	1.39
1	AA	1254	A	C5-C4	-6.34	1.34	1.38
1	AA	1285	A	C5-C4	-6.34	1.34	1.38
22	BA	63	A	C8-N7	6.34	1.35	1.31
22	BA	1528	A	C8-N7	6.34	1.35	1.31
1	AA	279	A	C8-N7	6.34	1.35	1.31
1	AA	59	A	C5-C4	-6.34	1.34	1.38
1	AA	1275	A	C8-N7	6.34	1.35	1.31
22	BA	508	A	N3-C4	6.34	1.38	1.34
22	BA	1668	A	N7-C5	-6.34	1.35	1.39
22	BA	2534	A	C5-C4	-6.34	1.34	1.38
1	AA	389	A	C8-N7	6.33	1.35	1.31
1	AA	1324	A	C5-C4	-6.33	1.34	1.38
22	BA	2183	A	C8-N7	6.33	1.35	1.31
1	AA	533	A	C5-C4	-6.33	1.34	1.38
22	BA	959	A	N7-C5	-6.33	1.35	1.39
1	AA	288	A	C5-C4	-6.33	1.34	1.38
1	AA	901	A	C5-C4	-6.33	1.34	1.38
22	BA	482	A	C5-C4	-6.33	1.34	1.38
1	AA	1117	A	C5-C4	-6.32	1.34	1.38
22	BA	165	A	C5-C4	-6.32	1.34	1.38
22	BA	391	A	N7-C5	-6.32	1.35	1.39
22	BA	1090	A	C8-N7	6.32	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1654	A	N7-C5	-6.32	1.35	1.39
22	BA	2225	A	N7-C5	-6.32	1.35	1.39
1	AA	687	A	C5-C4	-6.32	1.34	1.38
1	AA	938	A	C8-N7	6.32	1.35	1.31
22	BA	563	A	N9-C8	-6.32	1.32	1.37
22	BA	2273	A	N7-C5	-6.32	1.35	1.39
1	AA	300	A	N7-C5	-6.32	1.35	1.39
1	AA	602	A	C8-N7	6.32	1.35	1.31
1	AA	1394	A	C5-C4	-6.32	1.34	1.38
22	BA	1189	A	N7-C5	-6.32	1.35	1.39
23	BB	119	A	C8-N7	6.32	1.35	1.31
1	AA	655	A	C5-C4	-6.31	1.34	1.38
1	AA	263	A	C8-N7	6.31	1.35	1.31
1	AA	607	A	C5-C4	-6.31	1.34	1.38
1	AA	414	A	C5-C4	-6.31	1.34	1.38
22	BA	197	A	N7-C5	-6.31	1.35	1.39
22	BA	1901	A	N7-C5	-6.31	1.35	1.39
1	AA	152	A	C5-C4	-6.30	1.34	1.38
22	BA	362	A	N3-C4	6.30	1.38	1.34
22	BA	412	A	N7-C5	-6.30	1.35	1.39
22	BA	1214	A	N7-C5	-6.30	1.35	1.39
1	AA	1093	A	C8-N7	6.30	1.35	1.31
22	BA	2821	A	N7-C5	-6.30	1.35	1.39
1	AA	1271	A	C5-C4	-6.30	1.34	1.38
1	AA	1531	A	C8-N7	6.29	1.35	1.31
1	AA	300	A	C5-C4	-6.29	1.34	1.38
1	AA	718	A	C5-C4	-6.29	1.34	1.38
1	AA	1022	A	N3-C4	6.29	1.38	1.34
22	BA	1048	A	C8-N7	6.29	1.35	1.31
1	AA	371	A	C8-N7	6.29	1.35	1.31
22	BA	1020	A	N7-C5	-6.28	1.35	1.39
22	BA	2426	A	N7-C5	-6.28	1.35	1.39
1	AA	946	A	C8-N7	6.28	1.35	1.31
22	BA	1847	A	C5-C4	-6.28	1.34	1.38
1	AA	205	A	N3-C4	6.28	1.38	1.34
22	BA	1610	A	N7-C5	-6.28	1.35	1.39
22	BA	2267	A	N3-C4	6.28	1.38	1.34
22	BA	172	A	C8-N7	6.27	1.35	1.31
1	AA	382	A	C5-C4	-6.27	1.34	1.38
1	AA	621	A	C5-C4	-6.27	1.34	1.38
22	BA	1509	A	C5-C4	-6.27	1.34	1.38
22	BA	2430	A	C8-N7	6.27	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	635	A	C8-N7	6.27	1.35	1.31
22	BA	1776	G	C8-N7	-6.26	1.27	1.30
1	AA	98	A	C8-N7	6.26	1.35	1.31
1	AA	432	A	C8-N7	6.26	1.35	1.31
1	AA	663	A	C8-N7	6.26	1.35	1.31
1	AA	1275	A	C5-C4	-6.26	1.34	1.38
1	AA	1368	A	C8-N7	6.26	1.35	1.31
1	AA	1081	A	C8-N7	6.26	1.35	1.31
1	AA	1170	A	C5-C4	-6.25	1.34	1.38
22	BA	1591	A	C8-N7	6.25	1.35	1.31
1	AA	129	A	C5-C4	-6.25	1.34	1.38
22	BA	1495	A	C8-N7	6.25	1.35	1.31
1	AA	303	A	C8-N7	6.25	1.35	1.31
1	AA	149	A	C5-C4	-6.25	1.34	1.38
22	BA	2114	A	N3-C4	6.25	1.38	1.34
22	BA	1020	A	C5-C4	-6.25	1.34	1.38
22	BA	1744	A	C5-C4	-6.25	1.34	1.38
1	AA	151	A	C5-C4	-6.25	1.34	1.38
1	AA	1055	A	C8-N7	6.24	1.35	1.31
1	AA	1236	A	N3-C4	6.24	1.38	1.34
22	BA	960	A	N9-C8	-6.24	1.32	1.37
22	BA	1535	A	N3-C4	6.24	1.38	1.34
22	BA	1913	A	C5-C4	-6.24	1.34	1.38
1	AA	325	A	C5-C4	-6.24	1.34	1.38
1	AA	1319	A	C5-C4	-6.24	1.34	1.38
22	BA	1801	A	C5-C4	-6.24	1.34	1.38
22	BA	1365	A	N7-C5	-6.24	1.35	1.39
22	BA	716	A	C5-C4	-6.24	1.34	1.38
1	AA	915	A	C8-N7	6.23	1.35	1.31
1	AA	1288	A	C5-C4	-6.23	1.34	1.38
1	AA	1447	A	C5-C4	-6.23	1.34	1.38
22	BA	1129	A	N9-C8	-6.23	1.32	1.37
1	AA	1191	A	C5-C4	-6.22	1.34	1.38
22	BA	28	A	N7-C5	-6.22	1.35	1.39
22	BA	251	A	C5-C4	-6.22	1.34	1.38
22	BA	2095	A	C8-N7	6.22	1.35	1.31
22	BA	1745	A	C8-N7	6.22	1.35	1.31
1	AA	629	A	C5-C4	-6.22	1.34	1.38
1	AA	1493	A	C5-C4	-6.22	1.34	1.38
22	BA	1785	A	N7-C5	-6.22	1.35	1.39
1	AA	975	A	C5-C4	-6.21	1.34	1.38
22	BA	800	A	N7-C5	-6.21	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	160	A	C8-N7	6.21	1.35	1.31
1	AA	1362	A	C8-N7	6.21	1.35	1.31
22	BA	1505	A	C5-C4	-6.21	1.34	1.38
1	AA	860	A	C5-C4	-6.21	1.34	1.38
22	BA	1913	A	C8-N7	6.21	1.35	1.31
1	AA	172	A	C5-C4	-6.21	1.34	1.38
22	BA	422	A	N9-C8	-6.21	1.32	1.37
1	AA	482	A	C8-N7	6.21	1.35	1.31
22	BA	2335	A	N9-C8	-6.21	1.32	1.37
1	AA	1188	A	C5-C4	-6.20	1.34	1.38
22	BA	1505	A	C8-N7	6.20	1.35	1.31
1	AA	478	A	N3-C4	6.20	1.38	1.34
22	BA	1900	A	N9-C8	-6.20	1.32	1.37
22	BA	330	A	N7-C5	-6.20	1.35	1.39
22	BA	2687	U	C2-N3	-6.20	1.33	1.37
22	BA	1819	A	N7-C5	-6.19	1.35	1.39
22	BA	2709	G	C6-N1	-6.19	1.35	1.39
1	AA	1280	A	C5-C4	-6.19	1.34	1.38
22	BA	352	A	C5-C4	-6.19	1.34	1.38
22	BA	2183	A	N3-C4	6.19	1.38	1.34
1	AA	336	A	C8-N7	6.19	1.35	1.31
1	AA	1246	A	C5-C4	-6.19	1.34	1.38
22	BA	751	A	N9-C8	-6.19	1.32	1.37
1	AA	344	A	C5-C4	-6.18	1.34	1.38
22	BA	1669	A	N7-C5	-6.18	1.35	1.39
22	BA	2212	A	N7-C5	-6.18	1.35	1.39
22	BA	2592	G	N7-C5	-6.18	1.35	1.39
1	AA	1213	A	C5-C4	-6.18	1.34	1.38
22	BA	1802	A	N9-C8	-6.18	1.32	1.37
22	BA	1928	A	N7-C5	-6.18	1.35	1.39
22	BA	2328	A	N7-C5	-6.18	1.35	1.39
22	BA	849	A	N7-C5	-6.17	1.35	1.39
22	BA	2052	A	N7-C5	-6.17	1.35	1.39
1	AA	53	A	C8-N7	6.17	1.35	1.31
22	BA	482	A	N7-C5	-6.17	1.35	1.39
1	AA	994	A	C8-N7	6.17	1.35	1.31
22	BA	2799	A	C8-N7	6.17	1.35	1.31
1	AA	306	A	C5-C4	-6.17	1.34	1.38
1	AA	408	A	C5-C4	-6.17	1.34	1.38
22	BA	2792	A	C8-N7	6.17	1.35	1.31
22	BA	1885	A	C5-C4	-6.16	1.34	1.38
1	AA	1269	A	C5-C4	-6.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2191	A	C8-N7	6.16	1.35	1.31
1	AA	151	A	C8-N7	6.16	1.35	1.31
22	BA	348	A	C8-N7	6.16	1.35	1.31
1	AA	509	A	C8-N7	6.16	1.35	1.31
1	AA	1261	A	N3-C4	6.16	1.38	1.34
22	BA	526	A	N9-C8	-6.16	1.32	1.37
23	BB	66	A	C8-N7	6.16	1.35	1.31
22	BA	781	A	N7-C5	-6.15	1.35	1.39
1	AA	1055	A	C5-C4	-6.15	1.34	1.38
1	AA	1493	A	C8-N7	6.15	1.35	1.31
1	AA	452	A	C8-N7	6.15	1.35	1.31
1	AA	1117	A	C8-N7	6.15	1.35	1.31
22	BA	532	A	N7-C5	-6.15	1.35	1.39
1	AA	1225	A	C8-N7	6.14	1.35	1.31
22	BA	2147	A	N3-C4	6.14	1.38	1.34
1	AA	493	A	C5-C4	-6.14	1.34	1.38
22	BA	2565	A	N7-C5	-6.13	1.35	1.39
1	AA	1196	A	C5-C4	-6.13	1.34	1.38
22	BA	2799	A	N3-C4	6.13	1.38	1.34
1	AA	72	A	N3-C4	6.13	1.38	1.34
1	AA	1287	A	C5-C4	-6.12	1.34	1.38
22	BA	1363	C	N1-C6	-6.12	1.33	1.37
1	AA	1204	A	C5-C4	-6.12	1.34	1.38
22	BA	2005	A	N7-C5	-6.12	1.35	1.39
22	BA	2534	A	C8-N7	6.12	1.35	1.31
1	AA	983	A	C8-N7	6.12	1.35	1.31
1	AA	1180	A	C5-C4	-6.12	1.34	1.38
22	BA	699	A	N9-C8	-6.12	1.32	1.37
1	AA	1434	A	C8-N7	6.12	1.35	1.31
1	AA	749	A	C5-C4	-6.12	1.34	1.38
1	AA	831	A	C8-N7	6.12	1.35	1.31
22	BA	945	A	N9-C8	-6.12	1.32	1.37
22	BA	1321	A	N3-C4	6.12	1.38	1.34
23	BB	66	A	C5-C4	-6.12	1.34	1.38
22	BA	928	A	N7-C5	-6.12	1.35	1.39
1	AA	16	A	C8-N7	6.11	1.35	1.31
1	AA	1256	A	C5-C4	-6.11	1.34	1.38
22	BA	2654	A	C5-C4	-6.11	1.34	1.38
23	BB	58	A	C8-N7	6.11	1.35	1.31
55	B8	69	A	N3-C4	6.11	1.38	1.34
22	BA	1583	A	C5-C4	-6.11	1.34	1.38
1	AA	1374	A	C5-C4	-6.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1124	G	C5-C4	-6.11	1.34	1.38
1	AA	139	A	C5-C4	-6.11	1.34	1.38
22	BA	2067	G	C6-N1	-6.11	1.35	1.39
22	BA	1304	A	C8-N7	6.10	1.35	1.31
22	BA	2154	A	N3-C4	6.10	1.38	1.34
1	AA	1318	A	C5-C4	-6.10	1.34	1.38
22	BA	91	A	C8-N7	6.10	1.35	1.31
1	AA	563	A	C8-N7	6.10	1.35	1.31
1	AA	1201	A	N3-C4	6.10	1.38	1.34
1	AA	279	A	C5-C4	-6.10	1.34	1.38
22	BA	1515	A	C8-N7	6.10	1.35	1.31
22	BA	1787	A	N9-C8	-6.10	1.32	1.37
1	AA	373	A	C8-N7	6.09	1.35	1.31
1	AA	1179	A	C5-C4	-6.09	1.34	1.38
1	AA	1446	A	C5-C4	-6.09	1.34	1.38
23	BB	104	A	C8-N7	6.09	1.35	1.31
22	BA	10	A	C8-N7	6.09	1.35	1.31
23	BB	39	A	C5-C4	-6.09	1.34	1.38
22	BA	2587	A	N7-C5	-6.09	1.35	1.39
22	BA	2654	A	C8-N7	6.08	1.35	1.31
22	BA	1393	A	C8-N7	6.08	1.35	1.31
22	BA	1829	A	N9-C8	-6.08	1.32	1.37
1	AA	182	A	C8-N7	6.08	1.35	1.31
22	BA	844	A	C8-N7	6.08	1.35	1.31
1	AA	560	A	C8-N7	6.08	1.35	1.31
1	AA	968	A	C8-N7	6.08	1.35	1.31
1	AA	1176	A	C5-C4	-6.08	1.34	1.38
1	AA	1349	A	C8-N7	6.08	1.35	1.31
1	AA	1357	A	C5-C4	-6.08	1.34	1.38
22	BA	196	A	N9-C8	-6.08	1.32	1.37
1	AA	767	A	N7-C5	-6.08	1.35	1.39
22	BA	2749	A	C8-N7	6.08	1.35	1.31
1	AA	1252	A	C8-N7	6.07	1.35	1.31
22	BA	2433	A	N7-C5	-6.07	1.35	1.39
22	BA	2734	A	C8-N7	6.07	1.35	1.31
22	BA	94	A	C8-N7	6.07	1.35	1.31
22	BA	2199	A	N9-C8	-6.07	1.32	1.37
22	BA	1088	A	N3-C4	6.07	1.38	1.34
1	AA	977	A	C8-N7	6.06	1.35	1.31
1	AA	1000	A	N3-C4	6.06	1.38	1.34
1	AA	1046	A	C5-C4	-6.06	1.34	1.38
1	AA	236	A	C8-N7	6.06	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	204	A	N7-C5	-6.06	1.35	1.39
22	BA	781	A	N9-C8	-6.06	1.32	1.37
22	BA	2433	A	N9-C8	-6.06	1.32	1.37
22	BA	2856	A	C8-N7	6.06	1.35	1.31
1	AA	397	A	C5-C4	-6.06	1.34	1.38
22	BA	1039	A	C8-N7	6.06	1.35	1.31
22	BA	1508	A	N3-C4	6.06	1.38	1.34
1	AA	431	A	N3-C4	6.06	1.38	1.34
22	BA	2018	G	C8-N7	-6.06	1.27	1.30
1	AA	487	A	C5-C4	-6.05	1.34	1.38
1	AA	1227	A	C8-N7	6.05	1.35	1.31
22	BA	1591	A	N3-C4	6.05	1.38	1.34
22	BA	1046	A	N3-C4	6.05	1.38	1.34
22	BA	2711	A	N7-C5	-6.05	1.35	1.39
1	AA	430	A	C5-C4	-6.05	1.34	1.38
22	BA	2211	A	C5-C4	-6.05	1.34	1.38
22	BA	819	A	N7-C5	-6.05	1.35	1.39
22	BA	2278	A	N7-C5	-6.05	1.35	1.39
22	BA	203	A	N7-C5	-6.05	1.35	1.39
22	BA	1826	G	C5-C4	-6.05	1.34	1.38
1	AA	44	A	C5-C4	-6.04	1.34	1.38
1	AA	1225	A	C5-C4	-6.04	1.34	1.38
22	BA	368	A	C8-N7	6.04	1.35	1.31
22	BA	2199	A	N7-C5	-6.04	1.35	1.39
1	AA	3	A	C5-C4	-6.04	1.34	1.38
1	AA	1394	A	C8-N7	6.04	1.35	1.31
22	BA	2461	A	N7-C5	-6.04	1.35	1.39
1	AA	189	A	N3-C4	6.04	1.38	1.34
22	BA	899	A	C5-C4	-6.04	1.34	1.38
22	BA	1655	A	N9-C8	-6.04	1.32	1.37
22	BA	1028	A	N7-C5	-6.04	1.35	1.39
1	AA	51	A	C8-N7	6.04	1.35	1.31
1	AA	687	A	C8-N7	6.04	1.35	1.31
22	BA	2059	A	N7-C5	-6.04	1.35	1.39
1	AA	65	A	C5-C4	-6.04	1.34	1.38
1	AA	459	A	N3-C4	6.04	1.38	1.34
1	AA	498	A	N3-C4	6.04	1.38	1.34
1	AA	1171	A	C8-N7	6.04	1.35	1.31
23	BB	39	A	C8-N7	6.04	1.35	1.31
1	AA	968	A	C5-C4	-6.03	1.34	1.38
1	AA	1437	A	C8-N7	6.03	1.35	1.31
1	AA	415	A	N3-C4	6.03	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	119	A	C5-C4	-6.03	1.34	1.38
1	AA	298	A	C8-N7	6.03	1.35	1.31
1	AA	649	A	C5-C4	-6.03	1.34	1.38
22	BA	1073	A	N3-C4	6.03	1.38	1.34
22	BA	2366	A	N7-C5	-6.03	1.35	1.39
1	AA	1333	A	C8-N7	6.03	1.35	1.31
22	BA	125	A	C5-C4	-6.03	1.34	1.38
1	AA	1456	A	C5-C4	-6.02	1.34	1.38
22	BA	207	A	N7-C5	-6.02	1.35	1.39
1	AA	155	A	C5-C4	-6.02	1.34	1.38
1	AA	1350	A	C5-C4	-6.02	1.34	1.38
22	BA	223	A	N7-C5	-6.02	1.35	1.39
22	BA	2879	A	N7-C5	-6.02	1.35	1.39
22	BA	1746	A	C8-N7	6.02	1.35	1.31
1	AA	412	A	N3-C4	6.02	1.38	1.34
1	AA	495	A	C5-C4	-6.02	1.34	1.38
1	AA	1350	A	C8-N7	6.02	1.35	1.31
22	BA	1431	A	N7-C5	-6.02	1.35	1.39
1	AA	1170	A	C8-N7	6.01	1.35	1.31
1	AA	1229	A	C8-N7	6.01	1.35	1.31
1	AA	181	A	C5-C4	-6.01	1.34	1.38
22	BA	570	G	N1-C2	-6.01	1.32	1.37
22	BA	1968	G	C5-C4	-6.01	1.34	1.38
1	AA	1219	A	C5-C4	-6.01	1.34	1.38
22	BA	715	A	C8-N7	6.01	1.35	1.31
22	BA	1490	A	C5-C4	-6.01	1.34	1.38
1	AA	706	A	C5-C4	-6.01	1.34	1.38
1	AA	1531	A	C5-C4	-6.00	1.34	1.38
55	B8	14	A	N3-C4	6.00	1.38	1.34
22	BA	1502	A	C8-N7	6.00	1.35	1.31
1	AA	1	A	N3-C4	6.00	1.38	1.34
22	BA	447	A	N9-C8	-6.00	1.32	1.37
22	BA	752	A	C5-C4	-6.00	1.34	1.38
22	BA	1932	A	N7-C5	-6.00	1.35	1.39
1	AA	1492	A	C5-C4	-6.00	1.34	1.38
22	BA	1378	A	N7-C5	-6.00	1.35	1.39
1	AA	456	A	N3-C4	6.00	1.38	1.34
1	AA	560	A	C5-C4	-6.00	1.34	1.38
22	BA	933	A	C8-N7	6.00	1.35	1.31
22	BA	1912	A	C8-N7	6.00	1.35	1.31
1	AA	1169	A	C5-C4	-5.99	1.34	1.38
1	AA	55	A	C5-C4	-5.99	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	156	A	C8-N7	5.99	1.35	1.31
1	AA	1150	A	C5-C4	-5.99	1.34	1.38
22	BA	1494	A	C8-N7	5.99	1.35	1.31
22	BA	2660	A	C5-C4	-5.99	1.34	1.38
22	BA	1258	U	C2-N3	-5.99	1.33	1.37
22	BA	2718	G	C8-N7	-5.99	1.27	1.30
22	BA	2826	A	N7-C5	-5.99	1.35	1.39
1	AA	109	A	C8-N7	5.99	1.35	1.31
1	AA	630	A	C8-N7	5.99	1.35	1.31
1	AA	1507	A	C8-N7	5.99	1.35	1.31
22	BA	1735	A	C5-C4	-5.99	1.34	1.38
22	BA	960	A	N7-C5	-5.98	1.35	1.39
22	BA	294	A	C8-N7	5.98	1.35	1.31
22	BA	655	A	C8-N7	5.98	1.35	1.31
22	BA	1085	A	N3-C4	5.98	1.38	1.34
22	BA	1095	A	N3-C4	5.98	1.38	1.34
22	BA	575	A	N7-C5	-5.98	1.35	1.39
22	BA	2406	A	C8-N7	5.98	1.35	1.31
22	BA	2502	G	C5-C4	-5.98	1.34	1.38
22	BA	2781	A	N7-C5	-5.98	1.35	1.39
22	BA	508	A	C5-C4	-5.97	1.34	1.38
22	BA	1664	A	N7-C5	-5.97	1.35	1.39
22	BA	531	C	N3-C4	-5.97	1.29	1.33
22	BA	2451	A	C8-N7	5.97	1.35	1.31
22	BA	2757	A	N7-C5	-5.97	1.35	1.39
22	BA	1073	A	C8-N7	5.97	1.35	1.31
22	BA	1494	A	C5-C4	-5.97	1.34	1.38
22	BA	2311	A	C5-C4	-5.97	1.34	1.38
1	AA	1163	A	C5-C4	-5.97	1.34	1.38
22	BA	256	A	N7-C5	-5.97	1.35	1.39
22	BA	947	A	N7-C5	-5.97	1.35	1.39
1	AA	441	A	C8-N7	5.97	1.35	1.31
1	AA	1465	A	C8-N7	5.97	1.35	1.31
22	BA	1301	A	N7-C5	-5.97	1.35	1.39
1	AA	1092	A	C5-C4	-5.96	1.34	1.38
22	BA	2080	A	N9-C8	-5.96	1.32	1.37
1	AA	1398	A	C8-N7	5.96	1.35	1.31
22	BA	1054	A	N3-C4	5.96	1.38	1.34
22	BA	861	A	N7-C5	-5.96	1.35	1.39
1	AA	706	A	C8-N7	5.96	1.35	1.31
22	BA	716	A	C8-N7	5.96	1.35	1.31
22	BA	1522	A	C8-N7	5.96	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	825	A	N7-C5	-5.96	1.35	1.39
22	BA	2211	A	N3-C4	5.96	1.38	1.34
22	BA	2860	A	N7-C5	-5.96	1.35	1.39
1	AA	1201	A	C5-C4	-5.95	1.34	1.38
22	BA	2336	A	N7-C5	-5.95	1.35	1.39
1	AA	510	A	C8-N7	5.95	1.35	1.31
22	BA	146	A	C8-N7	5.95	1.35	1.31
22	BA	14	A	N7-C5	-5.95	1.35	1.39
1	AA	1413	A	C8-N7	5.95	1.35	1.31
1	AA	665	A	C8-N7	5.95	1.35	1.31
1	AA	19	A	C8-N7	5.95	1.35	1.31
22	BA	1614	A	N7-C5	-5.95	1.35	1.39
22	BA	2268	A	N7-C5	-5.95	1.35	1.39
1	AA	792	A	C8-N7	5.94	1.35	1.31
55	B8	59	A	N3-C4	5.94	1.38	1.34
1	AA	139	A	N3-C4	5.94	1.38	1.34
55	B8	66	A	N3-C4	5.94	1.38	1.34
1	AA	1016	A	C5-C4	-5.94	1.34	1.38
22	BA	2033	A	N7-C5	-5.93	1.35	1.39
22	BA	2335	A	N7-C5	-5.93	1.35	1.39
22	BA	2758	A	C8-N7	5.93	1.35	1.31
22	BA	1169	A	C8-N7	5.93	1.35	1.31
22	BA	2097	A	C5-C4	-5.93	1.34	1.38
22	BA	2497	A	N9-C8	-5.93	1.33	1.37
1	AA	825	A	C8-N7	5.93	1.35	1.31
22	BA	721	A	C8-N7	5.93	1.35	1.31
22	BA	878	A	C5-C4	-5.93	1.34	1.38
23	BB	59	A	C2-N3	5.93	1.38	1.33
22	BA	1204	A	C8-N7	5.93	1.35	1.31
1	AA	743	A	C8-N7	5.93	1.35	1.31
22	BA	529	A	C8-N7	5.93	1.35	1.31
22	BA	1014	A	C8-N7	5.93	1.35	1.31
22	BA	1286	A	N7-C5	-5.93	1.35	1.39
22	BA	1609	A	N7-C5	-5.93	1.35	1.39
1	AA	1324	A	C8-N7	5.92	1.35	1.31
22	BA	2314	A	C8-N7	5.92	1.35	1.31
22	BA	2662	A	C5-C4	-5.92	1.34	1.38
22	BA	1359	A	C8-N7	5.92	1.35	1.31
22	BA	453	A	N7-C5	-5.92	1.35	1.39
23	BB	53	A	C8-N7	5.92	1.35	1.31
1	AA	901	A	N7-C5	-5.92	1.35	1.39
22	BA	282	A	C5-C4	-5.92	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	196	A	C5-C4	-5.92	1.34	1.38
22	BA	1373	A	N7-C5	-5.92	1.35	1.39
22	BA	1668	A	N9-C8	-5.92	1.33	1.37
1	AA	383	A	C5-C4	-5.91	1.34	1.38
22	BA	1151	A	N7-C5	-5.91	1.35	1.39
1	AA	1014	A	C5-C4	-5.91	1.34	1.38
22	BA	449	A	N7-C5	-5.91	1.35	1.39
1	AA	1252	A	C5-C4	-5.90	1.34	1.38
22	BA	2799	A	C5-C4	-5.90	1.34	1.38
1	AA	1111	A	C5-C4	-5.90	1.34	1.38
22	BA	374	A	N7-C5	-5.90	1.35	1.39
22	BA	783	A	C5-C4	-5.90	1.34	1.38
22	BA	1551	A	N7-C5	-5.90	1.35	1.39
22	BA	2792	A	C5-C4	-5.90	1.34	1.38
1	AA	1012	A	N3-C4	5.90	1.38	1.34
22	BA	1147	A	C8-N7	5.90	1.35	1.31
22	BA	2184	A	N3-C4	5.89	1.38	1.34
1	AA	918	A	C8-N7	5.89	1.35	1.31
22	BA	570	G	N7-C5	-5.89	1.35	1.39
22	BA	722	A	C8-N7	5.89	1.35	1.31
22	BA	751	A	N7-C5	-5.89	1.35	1.39
22	BA	1376	C	N3-C4	-5.89	1.29	1.33
22	BA	83	A	C8-N7	5.89	1.35	1.31
22	BA	981	A	N9-C8	-5.89	1.33	1.37
22	BA	1525	A	C8-N7	5.88	1.35	1.31
1	AA	535	A	C8-N7	5.88	1.35	1.31
22	BA	104	A	C8-N7	5.88	1.35	1.31
22	BA	1927	A	N7-C5	-5.88	1.35	1.39
22	BA	2037	A	C5-C6	-5.88	1.35	1.41
1	AA	1146	A	C5-C4	-5.88	1.34	1.38
22	BA	808	G	N1-C2	-5.88	1.33	1.37
1	AA	1093	A	C5-C4	-5.88	1.34	1.38
22	BA	1272	A	N7-C5	-5.88	1.35	1.39
22	BA	1876	A	C5-C4	-5.88	1.34	1.38
1	AA	746	A	C8-N7	5.88	1.35	1.31
1	AA	1332	A	C5-C4	-5.88	1.34	1.38
22	BA	2873	A	N7-C5	-5.88	1.35	1.39
22	BA	1205	A	C8-N7	5.88	1.35	1.31
22	BA	1355	G	C5-C4	-5.88	1.34	1.38
23	BB	45	A	N3-C4	5.88	1.38	1.34
1	AA	238	A	C8-N7	5.87	1.35	1.31
1	AA	356	A	C8-N7	5.87	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1155	A	N3-C4	5.87	1.38	1.34
22	BA	2382	G	N7-C5	-5.87	1.35	1.39
1	AA	468	A	C5-C4	-5.87	1.34	1.38
22	BA	1253	A	C8-N7	5.87	1.35	1.31
22	BA	1508	A	C8-N7	5.87	1.35	1.31
22	BA	1848	A	C8-N7	5.87	1.35	1.31
22	BA	1593	A	C8-N7	5.87	1.35	1.31
1	AA	74	A	N3-C4	5.87	1.38	1.34
1	AA	1151	A	C5-C4	-5.87	1.34	1.38
22	BA	344	A	C8-N7	5.86	1.35	1.31
22	BA	501	A	N7-C5	-5.86	1.35	1.39
22	BA	983	A	N9-C8	-5.86	1.33	1.37
22	BA	1829	A	N7-C5	-5.86	1.35	1.39
22	BA	255	A	N7-C5	-5.86	1.35	1.39
22	BA	1744	A	C8-N7	5.86	1.35	1.31
1	AA	572	A	C8-N7	5.86	1.35	1.31
22	BA	2077	A	N9-C8	-5.86	1.33	1.37
22	BA	2409	G	N7-C5	-5.86	1.35	1.39
22	BA	2418	A	N7-C5	-5.86	1.35	1.39
22	BA	119	A	C8-N7	5.85	1.35	1.31
22	BA	1284	A	N7-C5	-5.85	1.35	1.39
23	BB	58	A	C5-C4	-5.85	1.34	1.38
22	BA	354	A	C5-C4	-5.85	1.34	1.38
22	BA	1637	A	N7-C5	-5.85	1.35	1.39
1	AA	1239	A	C5-C4	-5.85	1.34	1.38
22	BA	101	A	C5-C4	-5.85	1.34	1.38
22	BA	613	A	N3-C4	5.85	1.38	1.34
22	BA	1387	A	N7-C5	-5.85	1.35	1.39
22	BA	804	A	N7-C5	-5.84	1.35	1.39
55	B8	26	A	N3-C4	5.84	1.38	1.34
55	B8	58	A	N3-C4	5.84	1.38	1.34
1	AA	787	A	C8-N7	5.84	1.35	1.31
22	BA	512	G	N1-C2	-5.84	1.33	1.37
1	AA	430	A	C8-N7	5.84	1.35	1.31
1	AA	695	A	C8-N7	5.84	1.35	1.31
1	AA	1201	A	C8-N7	5.84	1.35	1.31
1	AA	143	A	C5-C4	-5.84	1.34	1.38
1	AA	1014	A	N3-C4	5.83	1.38	1.34
22	BA	1808	A	C8-N7	5.83	1.35	1.31
22	BA	1885	A	C8-N7	5.83	1.35	1.31
22	BA	2733	A	C8-N7	5.83	1.35	1.31
1	AA	728	A	C8-N7	5.83	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1428	A	C8-N7	5.83	1.35	1.31
1	AA	32	A	N3-C4	5.83	1.38	1.34
1	AA	975	A	C8-N7	5.83	1.35	1.31
1	AA	1191	A	C8-N7	5.83	1.35	1.31
22	BA	1413	A	C5-C4	-5.83	1.34	1.38
1	AA	596	A	C8-N7	5.82	1.35	1.31
22	BA	1029	A	N7-C5	-5.82	1.35	1.39
1	AA	814	A	N7-C5	-5.82	1.35	1.39
22	BA	2765	A	N7-C5	-5.82	1.35	1.39
55	B8	21	A	N3-C4	5.82	1.38	1.34
1	AA	1433	A	C8-N7	5.82	1.35	1.31
22	BA	345	A	C8-N7	5.82	1.35	1.31
22	BA	507	A	C5-C4	-5.82	1.34	1.38
22	BA	570	G	C6-N1	-5.82	1.35	1.39
22	BA	1384	A	N7-C5	-5.82	1.35	1.39
22	BA	1977	A	N9-C8	-5.82	1.33	1.37
1	AA	66	A	C8-N7	5.82	1.35	1.31
22	BA	2010	G	C6-N1	-5.82	1.35	1.39
22	BA	2134	A	N3-C4	5.82	1.38	1.34
1	AA	179	A	C5-C4	-5.81	1.34	1.38
1	AA	397	A	C8-N7	5.81	1.35	1.31
1	AA	167	A	C8-N7	5.81	1.35	1.31
22	BA	1144	A	N7-C5	-5.81	1.35	1.39
22	BA	1889	A	N7-C5	-5.81	1.35	1.39
1	AA	155	A	N3-C4	5.81	1.38	1.34
1	AA	560	A	N3-C4	5.81	1.38	1.34
1	AA	602	A	N3-C4	5.81	1.38	1.34
1	AA	1036	A	N3-C4	5.81	1.38	1.34
22	BA	1247	A	C8-N7	5.81	1.35	1.31
22	BA	1739	A	C5-C4	-5.80	1.34	1.38
22	BA	2066	C	N3-C4	-5.80	1.29	1.33
1	AA	872	A	C8-N7	5.80	1.35	1.31
1	AA	1238	A	N3-C4	5.80	1.38	1.34
22	BA	1676	A	N7-C5	-5.80	1.35	1.39
22	BA	1871	A	N3-C4	5.80	1.38	1.34
22	BA	1287	A	N9-C8	-5.79	1.33	1.37
1	AA	69	G	N9-C4	5.79	1.42	1.38
22	BA	94	A	C5-C4	-5.79	1.34	1.38
55	B8	51	A	N3-C4	5.79	1.38	1.34
22	BA	432	A	N7-C5	-5.79	1.35	1.39
22	BA	1571	A	N9-C8	-5.79	1.33	1.37
22	BA	2191	A	C5-C4	-5.79	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	167	A	N3-C4	5.78	1.38	1.34
55	B8	41	A	C5-C4	-5.78	1.34	1.38
1	AA	174	A	C5-C4	-5.78	1.34	1.38
1	AA	629	A	C8-N7	5.78	1.35	1.31
22	BA	2872	A	C8-N7	5.78	1.35	1.31
22	BA	160	A	C8-N7	5.78	1.35	1.31
22	BA	400	G	N7-C5	-5.78	1.35	1.39
22	BA	2670	A	C8-N7	5.78	1.35	1.31
1	AA	1374	A	C8-N7	5.78	1.35	1.31
22	BA	1853	A	N9-C8	-5.78	1.33	1.37
1	AA	523	A	C8-N7	5.78	1.35	1.31
22	BA	689	A	N7-C5	-5.78	1.35	1.39
22	BA	1579	A	C8-N7	5.78	1.35	1.31
22	BA	2471	A	C8-N7	5.78	1.35	1.31
22	BA	470	A	N7-C5	-5.77	1.35	1.39
22	BA	980	A	N9-C8	-5.77	1.33	1.37
22	BA	1077	A	N3-C4	5.77	1.38	1.34
1	AA	994	A	N3-C4	5.77	1.38	1.34
23	BB	46	A	C8-N7	5.77	1.35	1.31
22	BA	1187	G	C5-C4	-5.77	1.34	1.38
1	AA	313	A	C8-N7	5.76	1.35	1.31
1	AA	1375	A	C8-N7	5.76	1.35	1.31
1	AA	1157	A	C5-C4	-5.76	1.34	1.38
22	BA	515	A	N9-C8	-5.76	1.33	1.37
1	AA	1046	A	N3-C4	5.76	1.38	1.34
1	AA	19	A	N7-C5	-5.76	1.35	1.39
1	AA	487	A	C8-N7	5.76	1.35	1.31
1	AA	1250	A	C5-C4	-5.76	1.34	1.38
22	BA	668	A	N7-C5	-5.75	1.35	1.39
1	AA	353	A	C8-N7	5.75	1.35	1.31
22	BA	2267	A	N9-C8	-5.75	1.33	1.37
22	BA	2386	A	N9-C8	-5.75	1.33	1.37
22	BA	2566	A	C8-N7	5.75	1.35	1.31
22	BA	616	A	C8-N7	5.75	1.35	1.31
1	AA	1044	A	N3-C4	5.75	1.38	1.34
22	BA	125	A	N3-C4	5.75	1.38	1.34
1	AA	468	A	N3-C4	5.75	1.38	1.34
22	BA	1040	A	C8-N7	5.75	1.35	1.31
22	BA	1127	A	N7-C5	-5.75	1.35	1.39
22	BA	2686	G	C8-N7	-5.75	1.27	1.30
22	BA	2369	A	N7-C5	-5.74	1.35	1.39
22	BA	2723	C	N3-C4	-5.74	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2577	A	N9-C8	-5.74	1.33	1.37
1	AA	1410	A	C8-N7	5.74	1.35	1.31
22	BA	1046	A	C5-C4	-5.74	1.34	1.38
1	AA	262	A	C8-N7	5.74	1.35	1.31
1	AA	288	A	C8-N7	5.74	1.35	1.31
1	AA	498	A	C8-N7	5.74	1.35	1.31
1	AA	1004	A	N3-C4	5.74	1.38	1.34
22	BA	2741	A	N7-C5	-5.74	1.35	1.39
1	AA	1339	A	C8-N7	5.73	1.35	1.31
22	BA	1263	U	C2-N3	-5.73	1.33	1.37
1	AA	313	A	N7-C5	-5.73	1.35	1.39
22	BA	1067	A	N3-C4	5.73	1.38	1.34
22	BA	1103	A	N3-C4	5.73	1.38	1.34
22	BA	1711	A	N7-C5	-5.73	1.35	1.39
22	BA	2317	A	C8-N7	5.73	1.35	1.31
1	AA	502	A	C8-N7	5.73	1.35	1.31
22	BA	332	A	C8-N7	5.73	1.35	1.31
22	BA	566	U	C2-N3	-5.73	1.33	1.37
22	BA	905	A	C8-N7	5.73	1.35	1.31
23	BB	59	A	N3-C4	5.73	1.38	1.34
22	BA	2003	A	N7-C5	-5.73	1.35	1.39
22	BA	2061	G	C5-C4	-5.72	1.34	1.38
22	BA	2820	A	N3-C4	5.72	1.38	1.34
1	AA	71	A	C5-C4	-5.72	1.34	1.38
55	B8	6	A	N3-C4	5.72	1.38	1.34
22	BA	2063	C	N3-C4	-5.72	1.29	1.33
22	BA	727	A	N7-C5	-5.72	1.35	1.39
22	BA	2247	A	N9-C8	-5.72	1.33	1.37
22	BA	2309	A	N3-C4	5.72	1.38	1.34
22	BA	165	A	C8-N7	5.72	1.35	1.31
22	BA	1772	A	N9-C8	-5.72	1.33	1.37
1	AA	1257	A	N3-C4	5.72	1.38	1.34
22	BA	608	A	N9-C8	-5.71	1.33	1.37
1	AA	28	A	C8-N7	5.71	1.35	1.31
1	AA	130	A	N3-C4	5.71	1.38	1.34
22	BA	515	A	N7-C5	-5.71	1.35	1.39
22	BA	984	A	N9-C8	-5.71	1.33	1.37
22	BA	1353	A	N7-C5	-5.71	1.35	1.39
22	BA	1439	A	N7-C5	-5.71	1.35	1.39
1	AA	1246	A	N3-C4	5.71	1.38	1.34
22	BA	49	A	N9-C8	-5.71	1.33	1.37
22	BA	1264	A	N9-C8	-5.71	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	99	A	N7-C5	-5.71	1.35	1.39
22	BA	1583	A	N3-C4	5.71	1.38	1.34
22	BA	1949	G	N7-C5	-5.71	1.35	1.39
1	AA	1236	A	C8-N7	5.70	1.35	1.31
22	BA	218	A	N7-C5	-5.70	1.35	1.39
22	BA	1156	A	N9-C8	-5.70	1.33	1.37
22	BA	1342	A	N9-C8	-5.70	1.33	1.37
22	BA	1580	A	C8-N7	5.70	1.35	1.31
22	BA	2119	A	N3-C4	5.70	1.38	1.34
1	AA	937	A	C8-N7	5.70	1.35	1.31
1	AA	1080	A	C8-N7	5.70	1.35	1.31
22	BA	2868	A	N7-C5	-5.70	1.35	1.39
1	AA	270	A	C8-N7	5.70	1.35	1.31
22	BA	1552	A	N7-C5	-5.70	1.35	1.39
22	BA	1994	C	N3-C4	-5.70	1.29	1.33
22	BA	2688	G	C5-C4	-5.70	1.34	1.38
1	AA	320	A	C8-N7	5.70	1.35	1.31
22	BA	1395	A	C8-N7	5.70	1.35	1.31
22	BA	1134	A	C8-N7	5.70	1.35	1.31
22	BA	685	A	N9-C8	-5.70	1.33	1.37
22	BA	771	G	C5-C4	-5.70	1.34	1.38
1	AA	459	A	C5-C4	-5.69	1.34	1.38
1	AA	1152	A	N3-C4	5.69	1.38	1.34
22	BA	599	A	C8-N7	5.69	1.35	1.31
22	BA	2101	A	N3-C4	5.69	1.38	1.34
1	AA	1225	A	N3-C4	5.69	1.38	1.34
22	BA	1565	C	N3-C4	-5.69	1.29	1.33
22	BA	1790	C	N1-C6	-5.69	1.33	1.37
1	AA	223	A	N3-C4	5.69	1.38	1.34
22	BA	1143	A	N9-C8	-5.69	1.33	1.37
1	AA	270	A	N3-C4	5.69	1.38	1.34
1	AA	441	A	N3-C4	5.69	1.38	1.34
1	AA	996	A	C5-C4	-5.69	1.34	1.38
22	BA	199	A	C8-N7	5.69	1.35	1.31
22	BA	1272	A	N9-C8	-5.69	1.33	1.37
22	BA	1759	A	N7-C5	-5.69	1.35	1.39
22	BA	1679	A	N7-C5	-5.69	1.35	1.39
22	BA	1713	A	C8-N7	5.68	1.35	1.31
1	AA	648	A	C5-C4	-5.68	1.34	1.38
22	BA	103	A	C8-N7	5.68	1.35	1.31
22	BA	1098	A	C5-C4	-5.68	1.34	1.38
1	AA	465	A	N3-C4	5.68	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	366	A	C5-C4	-5.68	1.34	1.38
22	BA	443	A	N3-C4	5.68	1.38	1.34
22	BA	1717	A	C8-N7	5.68	1.35	1.31
1	AA	1102	A	C8-N7	5.68	1.35	1.31
22	BA	792	A	N9-C8	-5.68	1.33	1.37
1	AA	1396	A	N7-C5	-5.68	1.35	1.39
22	BA	144	A	C8-N7	5.68	1.35	1.31
1	AA	274	A	N3-C4	5.67	1.38	1.34
1	AA	460	A	C5-C4	-5.67	1.34	1.38
23	BB	104	A	N7-C5	-5.67	1.35	1.39
1	AA	583	A	C8-N7	5.67	1.35	1.31
1	AA	451	A	C5-C4	-5.67	1.34	1.38
22	BA	677	A	N7-C5	-5.67	1.35	1.39
22	BA	445	C	N3-C4	-5.67	1.29	1.33
1	AA	71	A	N3-C4	5.67	1.38	1.34
22	BA	27	G	N7-C5	-5.67	1.35	1.39
22	BA	2019	A	N7-C5	-5.67	1.35	1.39
22	BA	2284	A	N7-C5	-5.67	1.35	1.39
22	BA	1080	A	N3-C4	5.67	1.38	1.34
22	BA	1977	A	N7-C5	-5.67	1.35	1.39
22	BA	739	A	N7-C5	-5.67	1.35	1.39
1	AA	10	A	C8-N7	5.66	1.35	1.31
22	BA	342	A	C8-N7	5.66	1.35	1.31
1	AA	649	A	N3-C4	5.66	1.38	1.34
22	BA	1666	G	C5-C4	-5.66	1.34	1.38
22	BA	2176	A	N3-C4	5.66	1.38	1.34
1	AA	1502	A	N9-C8	-5.66	1.33	1.37
22	BA	936	A	C8-N7	5.66	1.35	1.31
22	BA	2886	A	C8-N7	5.66	1.35	1.31
22	BA	352	A	N3-C4	5.65	1.38	1.34
22	BA	1916	A	C8-N7	5.65	1.35	1.31
1	AA	498	A	C2-N3	5.65	1.38	1.33
1	AA	190	A	C8-N7	5.65	1.35	1.31
1	AA	493	A	N3-C4	5.65	1.38	1.34
1	AA	1431	A	C8-N7	5.65	1.35	1.31
22	BA	750	A	N9-C8	-5.65	1.33	1.37
22	BA	1156	A	N7-C5	-5.65	1.35	1.39
22	BA	1739	A	C8-N7	5.65	1.35	1.31
22	BA	845	A	C8-N7	5.64	1.35	1.31
22	BA	1778	U	C2-N3	-5.64	1.33	1.37
1	AA	3	A	N3-C4	5.64	1.38	1.34
22	BA	742	A	N7-C5	-5.64	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1597	A	C8-N7	5.64	1.35	1.31
1	AA	1012	A	C5-C4	-5.64	1.34	1.38
22	BA	447	A	N7-C5	-5.64	1.35	1.39
22	BA	2589	A	N9-C8	-5.64	1.33	1.37
1	AA	977	A	N3-C4	5.64	1.38	1.34
1	AA	958	A	N3-C4	5.64	1.38	1.34
1	AA	1248	A	N3-C4	5.63	1.38	1.34
1	AA	546	A	C8-N7	5.63	1.35	1.31
1	AA	1408	A	C8-N7	5.63	1.35	1.31
22	BA	191	A	N9-C8	-5.63	1.33	1.37
22	BA	1897	G	C6-N1	-5.63	1.35	1.39
22	BA	1966	A	N7-C5	-5.63	1.35	1.39
1	AA	702	A	C8-N7	5.63	1.35	1.31
22	BA	583	G	C5-C4	-5.63	1.34	1.38
22	BA	2634	A	C8-N7	5.63	1.35	1.31
22	BA	2564	A	N9-C8	-5.62	1.33	1.37
22	BA	2614	A	N9-C8	-5.62	1.33	1.37
22	BA	808	G	C6-N1	-5.62	1.35	1.39
22	BA	1001	A	N7-C5	-5.62	1.35	1.39
1	AA	1441	A	N3-C4	5.62	1.38	1.34
22	BA	2027	G	N7-C5	-5.62	1.35	1.39
22	BA	2469	A	C8-N7	5.62	1.35	1.31
22	BA	89	A	C8-N7	5.62	1.35	1.31
23	BB	78	A	N7-C5	-5.62	1.35	1.39
1	AA	1357	A	N3-C4	5.62	1.38	1.34
22	BA	1189	A	N9-C8	-5.62	1.33	1.37
22	BA	155	A	C8-N7	5.61	1.35	1.31
22	BA	1828	G	N9-C8	-5.61	1.33	1.37
22	BA	1787	A	C5-C6	-5.61	1.35	1.41
22	BA	2015	A	N9-C8	-5.61	1.33	1.37
22	BA	44	A	C8-N7	5.61	1.35	1.31
22	BA	1155	A	N9-C8	-5.61	1.33	1.37
1	AA	228	A	C8-N7	5.61	1.35	1.31
22	BA	49	A	N7-C5	-5.61	1.35	1.39
22	BA	340	A	C8-N7	5.61	1.35	1.31
22	BA	973	A	N7-C5	-5.61	1.35	1.39
22	BA	2018	G	C5-C4	-5.61	1.34	1.38
22	BA	374	A	N9-C8	-5.60	1.33	1.37
22	BA	513	A	C5-C6	-5.60	1.36	1.41
22	BA	1241	A	N7-C5	-5.60	1.35	1.39
22	BA	1749	A	C8-N7	5.60	1.35	1.31
22	BA	2722	G	C5-C4	-5.60	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	324	A	C8-N7	5.60	1.35	1.31
22	BA	1569	A	N9-C8	-5.60	1.33	1.37
22	BA	1848	A	N7-C5	-5.60	1.35	1.39
22	BA	1098	A	N3-C4	5.60	1.38	1.34
22	BA	1364	G	C5-C4	-5.60	1.34	1.38
22	BA	2020	A	N9-C8	-5.60	1.33	1.37
22	BA	1969	A	N9-C8	-5.59	1.33	1.37
22	BA	1930	G	C5-C4	-5.59	1.34	1.38
1	AA	1197	A	C8-N7	5.59	1.35	1.31
1	AA	1418	A	N7-C5	-5.59	1.35	1.39
22	BA	1679	A	N9-C8	-5.59	1.33	1.37
22	BA	2476	A	C8-N7	5.59	1.35	1.31
1	AA	374	A	N3-C4	5.59	1.38	1.34
22	BA	962	G	C5-C4	-5.59	1.34	1.38
22	BA	1134	A	N3-C4	5.59	1.38	1.34
22	BA	1383	A	C8-N7	5.59	1.35	1.31
22	BA	1987	A	N9-C8	-5.59	1.33	1.37
1	AA	553	A	C8-N7	5.58	1.35	1.31
23	BB	45	A	C5-C4	-5.58	1.34	1.38
22	BA	18	U	C2-N3	-5.58	1.33	1.37
22	BA	735	A	N7-C5	-5.58	1.35	1.39
22	BA	1260	A	N9-C8	-5.58	1.33	1.37
22	BA	1347	A	N7-C5	-5.58	1.35	1.39
22	BA	2270	A	N7-C5	-5.58	1.35	1.39
1	AA	98	A	N3-C4	5.58	1.38	1.34
22	BA	167	A	C8-N7	5.58	1.35	1.31
22	BA	219	A	N7-C5	-5.58	1.35	1.39
22	BA	2809	A	C8-N7	5.58	1.35	1.31
1	AA	1340	A	N3-C4	5.58	1.38	1.34
22	BA	310	A	C8-N7	5.58	1.35	1.31
1	AA	648	A	N3-C4	5.57	1.38	1.34
1	AA	1155	A	C5-C4	-5.57	1.34	1.38
22	BA	1469	A	N7-C5	-5.57	1.35	1.39
22	BA	1532	A	N3-C4	5.57	1.38	1.34
1	AA	344	A	N3-C4	5.57	1.38	1.34
22	BA	2045	C	N3-C4	-5.57	1.30	1.33
22	BA	2126	A	C5-C4	-5.57	1.34	1.38
22	BA	2459	A	N9-C8	-5.57	1.33	1.37
1	AA	696	A	N7-C5	-5.57	1.35	1.39
1	AA	1476	A	C8-N7	5.57	1.35	1.31
22	BA	753	A	N7-C5	-5.57	1.35	1.39
22	BA	1655	A	N7-C5	-5.57	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	496	A	N3-C4	5.56	1.38	1.34
22	BA	632	A	N9-C8	-5.56	1.33	1.37
22	BA	1477	A	N7-C5	-5.56	1.35	1.39
1	AA	1044	A	C5-C4	-5.56	1.34	1.38
1	AA	1219	A	C8-N7	5.56	1.35	1.31
55	B8	42	A	N3-C4	5.56	1.38	1.34
1	AA	642	A	C8-N7	5.56	1.35	1.31
22	BA	900	A	C5-C4	-5.56	1.34	1.38
1	AA	1441	A	C5-C4	-5.56	1.34	1.38
22	BA	1970	A	N9-C8	-5.56	1.33	1.37
22	BA	2060	A	N7-C5	-5.55	1.35	1.39
22	BA	2588	G	C6-N1	-5.55	1.35	1.39
1	AA	435	A	N3-C4	5.55	1.38	1.34
22	BA	1698	A	N7-C5	-5.55	1.35	1.39
22	BA	1722	A	C8-N7	5.55	1.35	1.31
55	B8	58	A	C5-C4	-5.55	1.34	1.38
1	AA	306	A	N3-C4	5.55	1.38	1.34
1	AA	1019	A	N3-C4	5.55	1.38	1.34
22	BA	1570	A	N9-C8	-5.55	1.33	1.37
22	BA	227	A	N9-C8	-5.55	1.33	1.37
22	BA	465	G	C8-N7	-5.55	1.27	1.30
1	AA	72	A	C5-C4	-5.55	1.34	1.38
22	BA	783	A	N3-C4	5.55	1.38	1.34
1	AA	448	A	N3-C4	5.54	1.38	1.34
1	AA	747	A	N3-C4	5.54	1.38	1.34
22	BA	397	U	C2-N3	-5.54	1.33	1.37
22	BA	979	A	C8-N7	5.54	1.35	1.31
22	BA	1900	A	N7-C5	-5.54	1.35	1.39
1	AA	1102	A	N3-C4	5.54	1.38	1.34
22	BA	428	A	N7-C5	-5.54	1.35	1.39
22	BA	1854	A	N9-C8	-5.54	1.33	1.37
22	BA	1088	A	C5-C4	-5.54	1.34	1.38
1	AA	383	A	N3-C4	5.54	1.38	1.34
1	AA	1152	A	C5-C4	-5.54	1.34	1.38
22	BA	1274	A	N7-C5	-5.54	1.35	1.39
22	BA	2065	C	N1-C6	-5.54	1.33	1.37
22	BA	2060	A	N9-C8	-5.54	1.33	1.37
1	AA	1248	A	C5-C4	-5.54	1.34	1.38
22	BA	278	A	C5-C4	-5.54	1.34	1.38
22	BA	1783	A	N7-C5	-5.54	1.35	1.39
22	BA	2026	U	C2-N3	-5.54	1.33	1.37
22	BA	899	A	N3-C4	5.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1084	A	C5-C4	-5.53	1.34	1.38
1	AA	1216	A	C5-C4	-5.53	1.34	1.38
22	BA	729	G	C8-N7	-5.53	1.27	1.30
1	AA	250	A	N3-C4	5.53	1.38	1.34
1	AA	452	A	C5-C4	-5.53	1.34	1.38
22	BA	38	A	N7-C5	-5.53	1.35	1.39
23	BB	66	A	N7-C5	-5.53	1.35	1.39
1	AA	559	A	C8-N7	5.53	1.35	1.31
22	BA	2448	A	N7-C5	-5.53	1.35	1.39
1	AA	640	A	C5-C4	-5.53	1.34	1.38
22	BA	1545	A	C8-N7	5.53	1.35	1.31
55	B8	38	A	C5-C4	-5.53	1.34	1.38
22	BA	2727	A	N9-C8	-5.52	1.33	1.37
1	AA	907	A	N7-C5	-5.52	1.35	1.39
22	BA	527	C	N1-C6	-5.52	1.33	1.37
22	BA	670	A	N7-C5	-5.52	1.35	1.39
22	BA	911	A	N7-C5	-5.52	1.35	1.39
22	BA	2719	G	C6-N1	-5.52	1.35	1.39
22	BA	1789	A	N9-C8	-5.52	1.33	1.37
22	BA	190	A	N9-C8	-5.52	1.33	1.37
22	BA	309	A	N9-C8	-5.52	1.33	1.37
22	BA	626	A	C8-N7	5.52	1.35	1.31
22	BA	2710	C	N3-C4	-5.52	1.30	1.33
1	AA	609	A	C8-N7	5.52	1.35	1.31
1	AA	1145	A	N3-C4	5.52	1.38	1.34
22	BA	2287	A	N7-C5	-5.52	1.35	1.39
1	AA	59	A	C8-N7	5.51	1.35	1.31
1	AA	983	A	N3-C4	5.51	1.38	1.34
1	AA	1082	A	C8-N7	5.51	1.35	1.31
22	BA	1095	A	C5-C4	-5.51	1.34	1.38
22	BA	2450	A	N7-C5	-5.51	1.35	1.39
22	BA	2588	G	N1-C2	-5.51	1.33	1.37
1	AA	630	A	N3-C4	5.51	1.38	1.34
1	AA	815	A	C8-N7	5.51	1.35	1.31
1	AA	864	A	C8-N7	5.51	1.35	1.31
22	BA	631	A	N7-C5	-5.51	1.35	1.39
22	BA	2816	G	C5-C4	-5.51	1.34	1.38
22	BA	1872	A	C5-C4	-5.51	1.34	1.38
22	BA	866	A	C8-N7	5.51	1.35	1.31
22	BA	2549	G	C6-N1	-5.51	1.35	1.39
22	BA	2550	G	C6-N1	-5.51	1.35	1.39
23	BB	45	A	C8-N7	5.51	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1324	A	N3-C4	5.50	1.38	1.34
22	BA	1265	A	N9-C8	-5.50	1.33	1.37
1	AA	461	A	N3-C4	5.50	1.38	1.34
1	AA	746	A	C5-C4	-5.50	1.34	1.38
22	BA	201	C	N3-C4	-5.50	1.30	1.33
22	BA	2565	A	N9-C8	-5.50	1.33	1.37
1	AA	1117	A	N3-C4	5.50	1.38	1.34
22	BA	346	A	N7-C5	-5.50	1.35	1.39
22	BA	2062	A	N7-C5	-5.50	1.35	1.39
22	BA	2572	A	N7-C5	-5.50	1.35	1.39
22	BA	5	A	C8-N7	5.50	1.35	1.31
22	BA	1070	A	C2-N3	5.50	1.38	1.33
22	BA	1085	A	C5-C4	-5.50	1.34	1.38
22	BA	454	A	N7-C5	-5.50	1.35	1.39
22	BA	1755	A	N7-C5	-5.50	1.35	1.39
22	BA	1847	A	C8-N7	5.50	1.35	1.31
22	BA	2407	A	N7-C5	-5.50	1.35	1.39
1	AA	315	A	C8-N7	5.49	1.35	1.31
22	BA	511	U	C2-N3	-5.49	1.33	1.37
22	BA	809	G	C8-N7	-5.49	1.27	1.30
22	BA	2070	A	N9-C8	-5.49	1.33	1.37
22	BA	161	A	C8-N7	5.49	1.35	1.31
22	BA	2205	A	C8-N7	5.49	1.35	1.31
1	AA	414	A	N3-C4	5.49	1.38	1.34
1	AA	1145	A	C5-C4	-5.49	1.34	1.38
22	BA	689	A	N9-C8	-5.49	1.33	1.37
22	BA	764	A	N7-C5	-5.49	1.35	1.39
22	BA	2547	A	C8-N7	5.49	1.35	1.31
1	AA	532	A	N3-C4	5.49	1.38	1.34
1	AA	975	A	N3-C4	5.49	1.38	1.34
22	BA	1237	A	N7-C5	-5.49	1.35	1.39
1	AA	964	A	C8-N7	5.49	1.35	1.31
1	AA	161	A	C8-N7	5.49	1.35	1.31
22	BA	1080	A	C5-C4	-5.49	1.34	1.38
22	BA	2198	A	C8-N7	5.49	1.35	1.31
1	AA	532	A	C5-C4	-5.48	1.34	1.38
1	AA	914	A	N7-C5	-5.48	1.35	1.39
22	BA	24	G	C6-N1	-5.48	1.35	1.39
22	BA	472	A	C8-N7	5.48	1.35	1.31
22	BA	483	A	N7-C5	-5.48	1.35	1.39
22	BA	534	U	C2-N3	-5.48	1.33	1.37
22	BA	577	G	C8-N7	-5.48	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1427	A	N9-C4	-5.48	1.34	1.37
1	AA	913	A	C8-N7	5.48	1.35	1.31
22	BA	834	G	C8-N7	-5.48	1.27	1.30
1	AA	1429	A	C8-N7	5.48	1.35	1.31
23	BB	57	A	C8-N7	5.48	1.35	1.31
1	AA	456	A	C5-C4	-5.48	1.34	1.38
22	BA	1532	A	C5-C4	-5.48	1.34	1.38
22	BA	1871	A	C5-C4	-5.48	1.34	1.38
22	BA	1872	A	N3-C4	5.48	1.38	1.34
1	AA	919	A	C8-N7	5.48	1.35	1.31
22	BA	586	A	N9-C8	-5.47	1.33	1.37
22	BA	2813	A	C8-N7	5.47	1.35	1.31
55	B8	21	A	C5-C4	-5.47	1.34	1.38
22	BA	925	A	C8-N7	5.47	1.35	1.31
22	BA	1262	A	N7-C5	-5.47	1.35	1.39
22	BA	1877	A	C8-N7	5.47	1.35	1.31
22	BA	2183	A	C5-C4	-5.47	1.34	1.38
22	BA	2657	A	C8-N7	5.47	1.35	1.31
22	BA	1866	A	C8-N7	5.47	1.35	1.31
1	AA	65	A	N3-C4	5.47	1.38	1.34
22	BA	541	A	N9-C8	-5.47	1.33	1.37
22	BA	1413	A	N3-C4	5.47	1.38	1.34
22	BA	1504	A	N3-C4	5.47	1.38	1.34
22	BA	2090	A	N9-C8	-5.47	1.33	1.37
22	BA	676	A	N9-C8	-5.47	1.33	1.37
22	BA	1434	A	N7-C5	-5.47	1.35	1.39
55	B8	42	A	C5-C4	-5.47	1.34	1.38
22	BA	5	A	N7-C5	-5.46	1.35	1.39
22	BA	538	A	C8-N7	5.46	1.35	1.31
22	BA	1165	A	C8-N7	5.46	1.35	1.31
1	AA	250	A	C5-C4	-5.46	1.34	1.38
1	AA	327	A	C8-N7	5.46	1.35	1.31
22	BA	1275	A	N9-C8	-5.46	1.33	1.37
22	BA	2435	A	N7-C5	-5.46	1.35	1.39
22	BA	2572	A	N9-C8	-5.46	1.33	1.37
1	AA	1196	A	N3-C4	5.46	1.38	1.34
22	BA	111	A	C8-N7	5.46	1.35	1.31
22	BA	682	G	C5-C4	-5.46	1.34	1.38
22	BA	2602	A	C5-C4	-5.46	1.34	1.38
55	B8	73	A	N3-C4	5.46	1.38	1.34
1	AA	59	A	N3-C4	5.46	1.38	1.34
55	B8	41	A	N3-C4	5.46	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	84	A	C8-N7	5.46	1.35	1.31
22	BA	1772	A	N7-C5	-5.46	1.35	1.39
22	BA	278	A	N3-C4	5.45	1.38	1.34
22	BA	1358	G	C6-N1	-5.45	1.35	1.39
22	BA	2619	C	N3-C4	-5.45	1.30	1.33
22	BA	1938	A	N7-C5	-5.45	1.35	1.39
1	AA	116	A	N7-C5	-5.45	1.35	1.39
22	BA	1299	G	C5-C4	-5.45	1.34	1.38
22	BA	1700	A	N7-C5	-5.45	1.35	1.39
22	BA	2288	A	N7-C5	-5.45	1.35	1.39
22	BA	2700	A	N7-C5	-5.45	1.35	1.39
22	BA	1338	G	C5-C4	-5.45	1.34	1.38
22	BA	2450	A	C5-C6	-5.45	1.36	1.41
1	AA	574	A	C8-N7	5.45	1.35	1.31
22	BA	2738	A	N9-C8	-5.45	1.33	1.37
1	AA	309	A	C8-N7	5.45	1.35	1.31
1	AA	364	A	C8-N7	5.45	1.35	1.31
22	BA	1269	A	N9-C8	-5.45	1.33	1.37
23	BB	15	A	N3-C4	5.44	1.38	1.34
1	AA	189	A	C5-C4	-5.44	1.34	1.38
1	AA	495	A	N3-C4	5.44	1.38	1.34
1	AA	1171	A	N3-C4	5.44	1.38	1.34
22	BA	1928	A	N9-C8	-5.44	1.33	1.37
1	AA	583	A	N7-C5	-5.44	1.35	1.39
22	BA	1111	A	N3-C4	5.44	1.38	1.34
1	AA	712	A	C8-N7	5.44	1.35	1.31
22	BA	213	A	N3-C4	5.44	1.38	1.34
22	BA	2810	A	C8-N7	5.44	1.35	1.31
22	BA	2887	A	N7-C5	-5.44	1.35	1.39
1	AA	465	A	C5-C4	-5.44	1.34	1.38
1	AA	908	A	C8-N7	5.43	1.35	1.31
22	BA	1299	G	C8-N7	-5.43	1.27	1.30
22	BA	1783	A	N9-C8	-5.43	1.33	1.37
22	BA	2227	A	C8-N7	5.43	1.35	1.31
22	BA	2688	G	C8-N7	-5.43	1.27	1.30
23	BB	99	A	N9-C8	-5.43	1.33	1.37
1	AA	2	A	N3-C4	5.43	1.38	1.34
22	BA	262	A	C8-N7	5.43	1.35	1.31
22	BA	1327	A	N7-C5	-5.43	1.35	1.39
1	AA	1285	A	N3-C4	5.43	1.38	1.34
22	BA	2071	A	N9-C8	-5.43	1.33	1.37
22	BA	330	A	N9-C8	-5.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	371	A	C8-N7	5.43	1.35	1.31
1	AA	608	A	C8-N7	5.43	1.35	1.31
22	BA	2212	A	C8-N7	5.43	1.35	1.31
1	AA	393	A	N3-C4	5.42	1.38	1.34
1	AA	1410	A	N3-C4	5.42	1.38	1.34
22	BA	2266	A	N9-C8	-5.42	1.33	1.37
22	BA	2547	A	N7-C5	-5.42	1.35	1.39
1	AA	190	A	C2-N3	5.42	1.38	1.33
1	AA	1169	A	N3-C4	5.42	1.38	1.34
1	AA	1219	A	N3-C4	5.42	1.38	1.34
1	AA	712	A	N3-C4	5.42	1.38	1.34
22	BA	239	C	N3-C4	-5.42	1.30	1.33
22	BA	1392	A	C8-N7	5.42	1.35	1.31
22	BA	1762	A	N7-C5	-5.42	1.35	1.39
22	BA	1824	G	N7-C5	-5.42	1.35	1.39
22	BA	2028	U	C2-N3	-5.42	1.33	1.37
1	AA	1019	A	C5-C4	-5.42	1.34	1.38
1	AA	909	A	C8-N7	5.42	1.35	1.31
1	AA	958	A	C5-C4	-5.42	1.34	1.38
22	BA	199	A	N7-C5	-5.42	1.35	1.39
22	BA	221	A	N7-C5	-5.42	1.35	1.39
22	BA	340	A	N7-C5	-5.42	1.36	1.39
22	BA	800	A	N9-C8	-5.42	1.33	1.37
55	B8	73	A	C5-C4	-5.42	1.34	1.38
1	AA	622	A	N3-C4	5.42	1.38	1.34
22	BA	2500	U	N3-C4	-5.42	1.33	1.38
1	AA	878	A	C8-N7	5.41	1.35	1.31
1	AA	1157	A	N3-C4	5.41	1.38	1.34
22	BA	101	A	C8-N7	5.41	1.35	1.31
22	BA	311	A	N7-C5	-5.41	1.36	1.39
1	AA	460	A	N3-C4	5.41	1.38	1.34
22	BA	2407	A	N9-C8	-5.41	1.33	1.37
1	AA	1000	A	C5-C4	-5.41	1.34	1.38
22	BA	354	A	N3-C4	5.41	1.38	1.34
22	BA	975	A	N9-C8	-5.41	1.33	1.37
22	BA	2266	A	N7-C5	-5.41	1.36	1.39
55	B8	76	A	C5-C4	-5.41	1.34	1.38
22	BA	1336	A	N7-C5	-5.41	1.36	1.39
1	AA	1274	A	N3-C4	5.41	1.38	1.34
22	BA	818	G	C8-N7	-5.41	1.27	1.30
22	BA	1230	A	C8-N7	5.40	1.35	1.31
22	BA	1393	A	N7-C5	-5.40	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1872	A	C8-N7	5.40	1.35	1.31
1	AA	190	A	N3-C4	5.40	1.38	1.34
1	AA	432	A	C5-C4	-5.40	1.34	1.38
22	BA	1918	A	C8-N7	5.40	1.35	1.31
1	AA	68	G	O3'-P	5.40	1.67	1.61
22	BA	1380	G	N9-C8	-5.40	1.34	1.37
22	BA	1650	A	N7-C5	-5.40	1.36	1.39
1	AA	949	A	C8-N7	5.40	1.35	1.31
22	BA	117	G	C5-C4	-5.40	1.34	1.38
1	AA	1171	A	C5-C4	-5.39	1.34	1.38
22	BA	1572	A	N7-C5	-5.39	1.36	1.39
22	BA	2598	A	N9-C8	-5.39	1.33	1.37
23	BB	79	G	C8-N7	-5.39	1.27	1.30
1	AA	321	A	C8-N7	5.39	1.35	1.31
22	BA	322	A	C8-N7	5.39	1.35	1.31
22	BA	1387	A	C8-N7	5.39	1.35	1.31
1	AA	431	A	C5-C4	-5.39	1.34	1.38
22	BA	764	A	N9-C8	-5.39	1.33	1.37
22	BA	2191	A	N3-C4	5.39	1.38	1.34
22	BA	529	A	N7-C5	-5.39	1.36	1.39
1	AA	1252	A	N3-C4	5.39	1.38	1.34
22	BA	71	A	C8-N7	5.39	1.35	1.31
22	BA	1858	A	C8-N7	5.39	1.35	1.31
1	AA	579	A	C8-N7	5.38	1.35	1.31
22	BA	173	A	C8-N7	5.38	1.35	1.31
22	BA	522	A	N9-C8	-5.38	1.33	1.37
22	BA	2392	A	N7-C5	-5.38	1.36	1.39
22	BA	2776	A	N9-C8	-5.38	1.33	1.37
55	B8	6	A	C5-C4	-5.38	1.34	1.38
22	BA	368	A	N3-C4	5.38	1.38	1.34
1	AA	466	A	N3-C4	5.38	1.38	1.34
1	AA	819	A	N3-C4	5.38	1.38	1.34
22	BA	1672	A	N7-C5	-5.38	1.36	1.39
22	BA	2049	G	N1-C2	-5.38	1.33	1.37
22	BA	2169	A	C2-N3	5.38	1.38	1.33
1	AA	430	A	N3-C4	5.38	1.38	1.34
22	BA	1395	A	N7-C5	-5.38	1.36	1.39
1	AA	1180	A	N3-C4	5.38	1.38	1.34
22	BA	1596	A	C8-N7	5.38	1.35	1.31
22	BA	2466	C	N3-C4	-5.38	1.30	1.33
22	BA	2753	A	C8-N7	5.38	1.35	1.31
23	BB	119	A	N3-C4	5.38	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	496	A	C5-C4	-5.38	1.34	1.38
1	AA	1430	A	C8-N7	5.38	1.35	1.31
23	BB	78	A	N9-C8	-5.38	1.33	1.37
1	AA	781	A	N9-C8	-5.38	1.33	1.37
22	BA	247	G	N9-C8	-5.37	1.34	1.37
22	BA	1008	A	N7-C5	-5.37	1.36	1.39
22	BA	1288	G	N7-C5	-5.37	1.36	1.39
1	AA	130	A	C8-N7	5.37	1.35	1.31
22	BA	402	A	C8-N7	5.37	1.35	1.31
22	BA	666	A	N7-C5	-5.37	1.36	1.39
22	BA	910	A	N7-C5	-5.37	1.36	1.39
22	BA	1010	A	N9-C8	-5.37	1.33	1.37
22	BA	2377	A	N7-C5	-5.37	1.36	1.39
22	BA	2418	A	N9-C8	-5.37	1.33	1.37
1	AA	1483	A	N7-C5	-5.37	1.36	1.39
55	B8	51	A	C5-C4	-5.37	1.34	1.38
1	AA	161	A	N3-C4	5.37	1.38	1.34
1	AA	978	A	N3-C4	5.37	1.38	1.34
23	BB	108	A	N7-C5	-5.37	1.36	1.39
1	AA	80	A	C2-N3	5.37	1.38	1.33
22	BA	53	A	N7-C5	-5.37	1.36	1.39
22	BA	1470	A	N7-C5	-5.37	1.36	1.39
22	BA	1899	A	N9-C8	-5.37	1.33	1.37
22	BA	582	A	N9-C8	-5.36	1.33	1.37
22	BA	2675	A	N9-C8	-5.36	1.33	1.37
1	AA	77	A	C5-C4	-5.36	1.34	1.38
22	BA	943	A	N7-C5	-5.36	1.36	1.39
22	BA	2693	G	C6-N1	-5.36	1.35	1.39
22	BA	2435	A	C6-N1	-5.36	1.31	1.35
22	BA	74	A	C8-N7	5.36	1.35	1.31
22	BA	1954	G	C5-C4	-5.36	1.34	1.38
22	BA	2443	C	N3-C4	-5.36	1.30	1.33
22	BA	2764	A	N7-C5	-5.36	1.36	1.39
22	BA	2750	A	C8-N7	5.36	1.35	1.31
22	BA	821	A	N9-C8	-5.35	1.33	1.37
22	BA	1385	A	N9-C8	-5.35	1.33	1.37
1	AA	746	A	N3-C4	5.35	1.38	1.34
22	BA	1276	A	N7-C5	-5.35	1.36	1.39
22	BA	1960	A	N7-C5	-5.35	1.36	1.39
1	AA	718	A	C8-N7	5.35	1.35	1.31
1	AA	780	A	N9-C8	-5.35	1.33	1.37
22	BA	661	A	N9-C8	-5.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	804	A	N9-C8	-5.35	1.33	1.37
22	BA	983	A	C5-C6	-5.35	1.36	1.41
22	BA	1000	A	N9-C8	-5.35	1.33	1.37
22	BA	2298	A	C8-N7	5.35	1.35	1.31
1	AA	1146	A	N3-C4	5.35	1.38	1.34
22	BA	155	A	N3-C4	5.35	1.38	1.34
22	BA	1186	G	N7-C5	-5.35	1.36	1.39
22	BA	2488	G	C6-N1	-5.35	1.35	1.39
1	AA	195	A	N3-C4	5.34	1.38	1.34
22	BA	2814	A	C8-N7	5.34	1.35	1.31
23	BB	59	A	N1-C2	5.34	1.39	1.34
1	AA	694	A	N3-C4	5.34	1.38	1.34
22	BA	231	A	N7-C5	-5.34	1.36	1.39
22	BA	690	G	C5-C4	-5.34	1.34	1.38
1	AA	1503	A	C8-N7	5.34	1.35	1.31
22	BA	1505	A	N3-C4	5.34	1.38	1.34
22	BA	2058	A	N7-C5	-5.34	1.36	1.39
22	BA	2450	A	N9-C8	-5.34	1.33	1.37
1	AA	608	A	N3-C4	5.34	1.38	1.34
1	AA	746	A	C2-N3	5.34	1.38	1.33
1	AA	1080	A	N7-C5	-5.34	1.36	1.39
22	BA	460	A	N7-C5	-5.34	1.36	1.39
22	BA	1009	A	N9-C8	-5.34	1.33	1.37
22	BA	1755	A	N9-C8	-5.34	1.33	1.37
22	BA	1815	A	N7-C5	-5.34	1.36	1.39
22	BA	2465	C	N3-C4	-5.34	1.30	1.33
22	BA	2501	C	N3-C4	-5.34	1.30	1.33
1	AA	32	A	C8-N7	5.33	1.35	1.31
1	AA	182	A	N3-C4	5.33	1.38	1.34
22	BA	400	G	C5-C4	-5.33	1.34	1.38
22	BA	1377	G	C6-N1	-5.33	1.35	1.39
22	BA	1393	A	N9-C8	-5.33	1.33	1.37
22	BA	2049	G	C6-N1	-5.33	1.35	1.39
1	AA	1216	A	N3-C4	5.33	1.38	1.34
22	BA	222	A	N9-C8	-5.33	1.33	1.37
22	BA	1966	A	N9-C8	-5.33	1.33	1.37
22	BA	2059	A	N9-C8	-5.33	1.33	1.37
22	BA	2899	A	N7-C5	-5.33	1.36	1.39
1	AA	1468	A	N7-C5	-5.33	1.36	1.39
22	BA	265	A	C8-N7	5.33	1.35	1.31
22	BA	637	A	C8-N7	5.33	1.35	1.31
22	BA	2061	G	N7-C5	-5.33	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2893	A	N7-C5	-5.33	1.36	1.39
1	AA	673	A	N3-C4	5.32	1.38	1.34
22	BA	1815	A	N9-C8	-5.32	1.33	1.37
1	AA	673	A	C8-N7	5.32	1.35	1.31
22	BA	799	G	C6-N1	-5.32	1.35	1.39
1	AA	205	A	C5-C4	-5.32	1.35	1.38
1	AA	978	A	C5-C4	-5.32	1.35	1.38
22	BA	1133	A	N9-C8	-5.32	1.33	1.37
22	BA	1828	G	C5-C4	-5.32	1.34	1.38
22	BA	943	A	N9-C8	-5.32	1.33	1.37
22	BA	2736	A	C8-N7	5.32	1.35	1.31
1	AA	675	A	C8-N7	5.32	1.35	1.31
1	AA	1179	A	N3-C4	5.32	1.38	1.34
22	BA	1175	A	C2-N3	5.32	1.38	1.33
22	BA	1848	A	C5-C4	-5.32	1.35	1.38
22	BA	2018	G	N9-C8	-5.32	1.34	1.37
1	AA	860	A	C8-N7	5.32	1.35	1.31
22	BA	1138	G	C5-C4	-5.32	1.34	1.38
22	BA	2495	G	C8-N7	-5.32	1.27	1.30
22	BA	2198	A	N7-C5	-5.31	1.36	1.39
55	B8	38	A	N3-C4	5.31	1.38	1.34
22	BA	28	A	N9-C8	-5.31	1.33	1.37
22	BA	572	A	N9-C8	-5.31	1.33	1.37
22	BA	1608	A	N3-C4	5.31	1.38	1.34
22	BA	1803	A	N9-C8	-5.31	1.33	1.37
22	BA	2882	A	C8-N7	5.31	1.35	1.31
22	BA	1567	G	N9-C8	-5.31	1.34	1.37
22	BA	2378	A	C8-N7	5.31	1.35	1.31
22	BA	2518	A	N7-C5	-5.31	1.36	1.39
1	AA	338	A	C8-N7	5.31	1.35	1.31
1	AA	938	A	N7-C5	-5.31	1.36	1.39
22	BA	1544	A	C8-N7	5.31	1.35	1.31
22	BA	1586	A	C5-C4	-5.31	1.35	1.38
22	BA	1805	A	N9-C8	-5.31	1.33	1.37
22	BA	346	A	C8-N7	5.31	1.35	1.31
22	BA	1952	A	N7-C5	-5.31	1.36	1.39
22	BA	502	A	N7-C5	-5.31	1.36	1.39
22	BA	2761	A	C8-N7	5.31	1.35	1.31
23	BB	73	A	N3-C4	5.31	1.38	1.34
22	BA	671	C	N3-C4	-5.30	1.30	1.33
22	BA	1919	A	C8-N7	5.30	1.35	1.31
22	BA	2352	A	N7-C5	-5.30	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2725	A	N7-C5	-5.30	1.36	1.39
22	BA	2322	A	N7-C5	-5.30	1.36	1.39
1	AA	559	A	N7-C5	-5.30	1.36	1.39
22	BA	1275	A	N7-C5	-5.30	1.36	1.39
22	BA	2327	A	N7-C5	-5.30	1.36	1.39
1	AA	143	A	N3-C4	5.30	1.38	1.34
1	AA	747	A	C5-C4	-5.30	1.35	1.38
1	AA	1236	A	N7-C5	-5.30	1.36	1.39
22	BA	570	G	C8-N7	-5.30	1.27	1.30
22	BA	825	A	N9-C8	-5.30	1.33	1.37
22	BA	1496	A	N7-C5	-5.30	1.36	1.39
22	BA	1626	A	C8-N7	5.30	1.35	1.31
1	AA	1534	A	C2-N3	5.30	1.38	1.33
22	BA	73	A	N7-C5	-5.30	1.36	1.39
22	BA	705	A	N9-C8	-5.30	1.33	1.37
22	BA	2513	A	N7-C5	-5.30	1.36	1.39
22	BA	1086	A	N3-C4	5.30	1.38	1.34
22	BA	2176	A	C5-C4	-5.30	1.35	1.38
1	AA	906	A	C8-N7	5.29	1.35	1.31
22	BA	927	A	C8-N7	5.29	1.35	1.31
1	AA	223	A	C5-C4	-5.29	1.35	1.38
1	AA	766	A	C8-N7	5.29	1.35	1.31
22	BA	53	A	C8-N7	5.29	1.35	1.31
22	BA	300	A	C8-N7	5.29	1.35	1.31
22	BA	430	A	C8-N7	5.29	1.35	1.31
22	BA	585	G	C8-N7	-5.29	1.27	1.30
22	BA	676	A	N7-C5	-5.29	1.36	1.39
22	BA	770	G	C6-N1	-5.29	1.35	1.39
22	BA	2726	A	N7-C5	-5.29	1.36	1.39
22	BA	1590	A	N3-C4	5.29	1.38	1.34
22	BA	2358	A	N9-C8	-5.29	1.33	1.37
1	AA	1042	A	C5-C4	-5.29	1.35	1.38
22	BA	794	A	N9-C8	-5.29	1.33	1.37
22	BA	2003	A	N9-C8	-5.29	1.33	1.37
1	AA	1513	A	N7-C5	-5.29	1.36	1.39
22	BA	2412	A	N7-C5	-5.29	1.36	1.39
22	BA	2829	A	N9-C8	-5.29	1.33	1.37
22	BA	603	A	C8-N7	5.28	1.35	1.31
22	BA	2067	G	N1-C2	-5.28	1.33	1.37
1	AA	784	A	C8-N7	5.28	1.35	1.31
22	BA	226	A	N7-C5	-5.28	1.36	1.39
22	BA	1794	A	N7-C5	-5.28	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2540	C	N3-C4	-5.28	1.30	1.33
1	AA	996	A	N3-C4	5.28	1.38	1.34
22	BA	577	G	C6-N1	-5.28	1.35	1.39
22	BA	1819	A	N9-C8	-5.28	1.33	1.37
22	BA	1357	C	N3-C4	-5.28	1.30	1.33
22	BA	251	A	N7-C5	-5.28	1.36	1.39
22	BA	2515	C	N1-C6	-5.28	1.33	1.37
22	BA	2521	C	N3-C4	-5.28	1.30	1.33
1	AA	448	A	C5-C4	-5.27	1.35	1.38
1	AA	964	A	N3-C4	5.27	1.38	1.34
22	BA	471	A	N7-C5	-5.27	1.36	1.39
22	BA	1057	A	N3-C4	5.27	1.38	1.34
1	AA	451	A	N3-C4	5.27	1.38	1.34
22	BA	631	A	N9-C8	-5.27	1.33	1.37
22	BA	1067	A	C5-C4	-5.27	1.35	1.38
22	BA	1336	A	N9-C8	-5.27	1.33	1.37
1	AA	802	A	N7-C5	-5.27	1.36	1.39
1	AA	101	A	N3-C4	5.27	1.38	1.34
1	AA	452	A	N3-C4	5.27	1.38	1.34
22	BA	1272	A	N3-C4	5.27	1.38	1.34
22	BA	1690	A	C8-N7	5.27	1.35	1.31
22	BA	2873	A	N9-C8	-5.27	1.33	1.37
1	AA	98	A	C5-C4	-5.27	1.35	1.38
1	AA	1016	A	N3-C4	5.27	1.38	1.34
22	BA	1054	A	C2-N3	5.27	1.38	1.33
22	BA	1226	A	N9-C8	-5.27	1.33	1.37
22	BA	2184	A	C5-C4	-5.27	1.35	1.38
1	AA	172	A	N3-C4	5.26	1.38	1.34
1	AA	704	A	N3-C4	5.26	1.38	1.34
1	AA	1480	A	C8-N7	5.26	1.35	1.31
22	BA	578	G	C8-N7	-5.26	1.27	1.30
22	BA	2038	G	N1-C2	-5.26	1.33	1.37
22	BA	2079	U	C2-N3	-5.26	1.34	1.37
22	BA	2432	A	N7-C5	-5.26	1.36	1.39
22	BA	196	A	N7-C5	-5.26	1.36	1.39
22	BA	2065	C	N3-C4	-5.26	1.30	1.33
1	AA	196	A	N3-C4	5.26	1.38	1.34
22	BA	734	A	N7-C5	-5.25	1.36	1.39
22	BA	821	A	N7-C5	-5.25	1.36	1.39
22	BA	189	G	C5-C4	-5.25	1.34	1.38
22	BA	423	A	N7-C5	-5.25	1.36	1.39
23	BB	29	A	C8-N7	5.25	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1021	A	C5-C4	-5.25	1.35	1.38
1	AA	1275	A	N3-C4	5.25	1.38	1.34
22	BA	505	A	N9-C8	-5.25	1.33	1.37
22	BA	2381	A	N7-C5	-5.25	1.36	1.39
22	BA	479	A	C8-N7	5.25	1.35	1.31
22	BA	788	A	N9-C8	-5.25	1.33	1.37
22	BA	1073	A	C2-N3	5.25	1.38	1.33
22	BA	1596	A	N7-C5	-5.25	1.36	1.39
22	BA	311	A	C8-N7	5.25	1.35	1.31
22	BA	2298	A	N3-C4	5.25	1.38	1.34
22	BA	2531	A	C8-N7	5.25	1.35	1.31
55	B8	14	A	C5-C4	-5.25	1.35	1.38
1	AA	1022	A	C5-C4	-5.24	1.35	1.38
22	BA	64	A	C8-N7	5.24	1.35	1.31
22	BA	706	A	N7-C5	-5.24	1.36	1.39
22	BA	829	A	N7-C5	-5.24	1.36	1.39
22	BA	946	C	N3-C4	-5.24	1.30	1.33
22	BA	2448	A	N9-C8	-5.24	1.33	1.37
1	AA	461	A	C5-C4	-5.24	1.35	1.38
1	AA	1004	A	C5-C4	-5.24	1.35	1.38
1	AA	1289	A	N3-C4	5.24	1.38	1.34
22	BA	1847	A	N7-C5	-5.24	1.36	1.39
22	BA	1913	A	N3-C4	5.24	1.38	1.34
22	BA	2799	A	C2-N3	5.24	1.38	1.33
1	AA	1531	A	N3-C4	5.24	1.38	1.34
22	BA	2333	A	N7-C5	-5.24	1.36	1.39
22	BA	2513	A	N9-C8	-5.24	1.33	1.37
22	BA	621	A	N7-C5	-5.24	1.36	1.39
22	BA	1735	A	N3-C4	5.24	1.38	1.34
22	BA	577	G	C5-C4	-5.24	1.34	1.38
22	BA	585	G	C6-N1	-5.24	1.35	1.39
22	BA	1096	A	C2-N3	5.24	1.38	1.33
22	BA	2244	U	C2-N3	-5.24	1.34	1.37
22	BA	2425	A	N9-C8	-5.24	1.33	1.37
22	BA	1363	C	N3-C4	-5.23	1.30	1.33
22	BA	2247	A	N7-C5	-5.23	1.36	1.39
23	BB	58	A	N3-C4	5.23	1.38	1.34
1	AA	974	A	N3-C4	5.23	1.38	1.34
1	AA	1500	A	N9-C8	-5.23	1.33	1.37
22	BA	270	A	C8-N7	5.23	1.35	1.31
22	BA	282	A	N3-C4	5.23	1.38	1.34
22	BA	478	A	C8-N7	5.23	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1286	A	C8-N7	5.23	1.35	1.31
1	AA	397	A	N3-C4	5.23	1.38	1.34
1	AA	729	A	C8-N7	5.23	1.35	1.31
22	BA	586	A	N7-C5	-5.23	1.36	1.39
22	BA	602	A	C8-N7	5.23	1.35	1.31
22	BA	1784	A	N9-C8	-5.23	1.33	1.37
22	BA	2002	G	C6-N1	-5.23	1.35	1.39
1	AA	1274	A	C5-C4	-5.23	1.35	1.38
22	BA	2792	A	N3-C4	5.23	1.38	1.34
25	BD	152	PRO	CG-CD	-5.23	1.33	1.50
1	AA	923	A	C8-N7	5.23	1.35	1.31
1	AA	923	A	N7-C5	-5.23	1.36	1.39
22	BA	1048	A	N3-C4	5.23	1.38	1.34
22	BA	1810	A	N9-C8	-5.23	1.33	1.37
23	BB	59	A	C8-N7	5.23	1.35	1.31
23	BB	79	G	N7-C5	-5.23	1.36	1.39
1	AA	1299	A	C5-C4	-5.23	1.35	1.38
1	AA	1375	A	N3-C4	5.23	1.38	1.34
22	BA	1890	A	N7-C5	-5.23	1.36	1.39
22	BA	127	A	N7-C5	-5.22	1.36	1.39
22	BA	528	A	N9-C8	-5.22	1.33	1.37
1	AA	781	A	N7-C5	-5.22	1.36	1.39
22	BA	541	A	N7-C5	-5.22	1.36	1.39
22	BA	1367	A	N7-C5	-5.22	1.36	1.39
22	BA	1197	G	C5-C4	-5.22	1.34	1.38
22	BA	1427	A	N7-C5	-5.22	1.36	1.39
22	BA	1503	A	N3-C4	5.22	1.38	1.34
1	AA	892	A	C8-N7	5.22	1.35	1.31
22	BA	71	A	N3-C4	5.22	1.38	1.34
22	BA	538	A	N3-C4	5.22	1.38	1.34
22	BA	863	A	N9-C8	-5.22	1.33	1.37
22	BA	1905	C	N1-C6	-5.22	1.34	1.37
1	AA	1167	A	N3-C4	5.22	1.38	1.34
22	BA	1157	G	C8-N7	-5.22	1.27	1.30
22	BA	1966	A	C8-N7	5.22	1.35	1.31
22	BA	1981	A	N7-C5	-5.22	1.36	1.39
22	BA	964	C	N3-C4	-5.21	1.30	1.33
22	BA	1371	G	C6-N1	-5.21	1.35	1.39
1	AA	205	A	C2-N3	5.21	1.38	1.33
22	BA	789	A	N3-C4	5.21	1.38	1.34
22	BA	1877	A	N3-C4	5.21	1.38	1.34
1	AA	1257	A	C5-C4	-5.21	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	860	U	C2-N3	-5.21	1.34	1.37
22	BA	1509	A	N3-C4	5.21	1.38	1.34
22	BA	2171	A	C2-N3	5.21	1.38	1.33
22	BA	439	A	C8-N7	5.21	1.35	1.31
22	BA	1477	A	N9-C8	-5.21	1.33	1.37
22	BA	2158	A	C2-N3	5.21	1.38	1.33
22	BA	2850	A	N9-C8	-5.21	1.33	1.37
22	BA	95	A	C8-N7	5.21	1.35	1.31
22	BA	477	A	N7-C5	-5.21	1.36	1.39
22	BA	692	C	N3-C4	-5.21	1.30	1.33
55	B8	26	A	C5-C4	-5.21	1.35	1.38
1	AA	792	A	N3-C4	5.21	1.38	1.34
1	AA	1513	A	N9-C8	-5.21	1.33	1.37
22	BA	532	A	N9-C8	-5.21	1.33	1.37
1	AA	408	A	N3-C4	5.20	1.38	1.34
1	AA	415	A	C5-C4	-5.20	1.35	1.38
1	AA	162	A	C8-N7	5.20	1.35	1.31
1	AA	579	A	N7-C5	-5.20	1.36	1.39
22	BA	1677	A	N9-C8	-5.20	1.33	1.37
22	BA	1987	A	N7-C5	-5.20	1.36	1.39
22	BA	1998	A	N7-C5	-5.20	1.36	1.39
22	BA	996	A	N7-C5	-5.20	1.36	1.39
22	BA	2726	A	N9-C8	-5.20	1.33	1.37
22	BA	2872	A	N7-C5	-5.20	1.36	1.39
22	BA	1194	A	N9-C8	-5.20	1.33	1.37
22	BA	1993	U	C2-N3	-5.20	1.34	1.37
22	BA	1089	A	C2-N3	5.20	1.38	1.33
22	BA	1548	A	N7-C5	-5.20	1.36	1.39
22	BA	2094	A	N7-C5	-5.20	1.36	1.39
22	BA	2097	A	N3-C4	5.20	1.38	1.34
22	BA	2595	G	N1-C2	-5.20	1.33	1.37
1	AA	694	A	C8-N7	5.19	1.35	1.31
22	BA	2758	A	N9-C8	-5.19	1.33	1.37
1	AA	595	A	N3-C4	5.19	1.38	1.34
22	BA	2588	G	C8-N7	-5.19	1.27	1.30
22	BA	2766	A	N3-C4	5.19	1.38	1.34
22	BA	523	C	N3-C4	-5.19	1.30	1.33
22	BA	2478	A	C8-N7	5.19	1.35	1.31
22	BA	223	A	C8-N7	5.19	1.35	1.31
22	BA	1153	C	N3-C4	-5.19	1.30	1.33
22	BA	1937	A	N9-C8	-5.19	1.33	1.37
22	BA	2461	A	N9-C8	-5.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	251	A	N3-C4	5.19	1.38	1.34
22	BA	1549	A	N9-C8	-5.19	1.33	1.37
22	BA	2212	A	N9-C8	-5.19	1.33	1.37
24	BC	231	PRO	CG-CD	-5.19	1.33	1.50
22	BA	149	A	N7-C5	-5.19	1.36	1.39
1	AA	687	A	N3-C4	5.18	1.38	1.34
1	AA	968	A	N3-C4	5.18	1.38	1.34
1	AA	1396	A	C8-N7	5.18	1.35	1.31
22	BA	793	A	N9-C8	-5.18	1.33	1.37
22	BA	1144	A	N9-C8	-5.18	1.33	1.37
22	BA	2038	G	C8-N7	-5.18	1.27	1.30
22	BA	2330	G	C5-C4	-5.18	1.34	1.38
1	AA	1005	A	C2-N3	5.18	1.38	1.33
22	BA	131	A	N9-C8	-5.18	1.33	1.37
22	BA	1690	A	N7-C5	-5.18	1.36	1.39
26	BE	76	PRO	CG-CD	-5.18	1.33	1.50
1	AA	374	A	C8-N7	5.18	1.35	1.31
22	BA	1664	A	N9-C8	-5.18	1.33	1.37
22	BA	2042	A	N9-C8	-5.18	1.33	1.37
22	BA	2135	A	C2-N3	5.18	1.38	1.33
22	BA	2411	A	N7-C5	-5.18	1.36	1.39
22	BA	1048	A	C5-C4	-5.17	1.35	1.38
22	BA	654	A	C2-N3	5.17	1.38	1.33
1	AA	1306	A	N3-C4	5.17	1.38	1.34
22	BA	574	A	N9-C8	-5.17	1.33	1.37
22	BA	1678	A	N9-C8	-5.17	1.33	1.37
22	BA	1793	C	N3-C4	-5.17	1.30	1.33
22	BA	2029	G	C5-C4	-5.17	1.34	1.38
22	BA	2281	A	N7-C5	-5.17	1.36	1.39
22	BA	2524	G	C6-N1	-5.17	1.35	1.39
22	BA	2639	A	N3-C4	5.17	1.38	1.34
22	BA	320	A	C8-N7	5.17	1.35	1.31
22	BA	2033	A	C8-N7	5.17	1.35	1.31
23	BB	109	A	N7-C5	-5.17	1.36	1.39
1	AA	1081	A	N3-C4	5.17	1.38	1.34
22	BA	743	A	N7-C5	-5.17	1.36	1.39
22	BA	2814	A	N7-C5	-5.17	1.36	1.39
1	AA	1170	A	N3-C4	5.17	1.38	1.34
1	AA	1188	A	N3-C4	5.17	1.38	1.34
22	BA	2632	A	N9-C8	-5.17	1.33	1.37
22	BA	101	A	N3-C4	5.16	1.38	1.34
22	BA	432	A	N9-C8	-5.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2437	G	C5-C4	-5.16	1.34	1.38
22	BA	2757	A	N9-C8	-5.16	1.33	1.37
1	AA	523	A	N3-C4	5.16	1.38	1.34
1	AA	1299	A	N3-C4	5.16	1.38	1.34
22	BA	1871	A	C2-N3	5.16	1.38	1.33
1	AA	959	A	N3-C4	5.16	1.38	1.34
22	BA	501	A	N9-C8	-5.16	1.33	1.37
1	AA	1239	A	N3-C4	5.16	1.38	1.34
22	BA	1008	A	C8-N7	5.16	1.35	1.31
1	AA	412	A	C5-C4	-5.16	1.35	1.38
22	BA	19	A	N7-C5	-5.16	1.36	1.39
22	BA	990	A	N7-C5	-5.15	1.36	1.39
1	AA	1374	A	N3-C4	5.15	1.38	1.34
22	BA	412	A	N9-C8	-5.15	1.33	1.37
22	BA	2378	A	N7-C5	-5.15	1.36	1.39
22	BA	1244	A	C8-N7	5.15	1.35	1.31
22	BA	2336	A	N9-C8	-5.15	1.33	1.37
22	BA	362	A	C5-C4	-5.15	1.35	1.38
22	BA	483	A	C8-N7	5.15	1.35	1.31
22	BA	527	C	N3-C4	-5.15	1.30	1.33
22	BA	2588	G	C5-C4	-5.15	1.34	1.38
22	BA	1667	G	N7-C5	-5.15	1.36	1.39
22	BA	971	G	C8-N7	-5.14	1.27	1.30
22	BA	1919	A	N7-C5	-5.14	1.36	1.39
22	BA	2053	G	C5-C4	-5.14	1.34	1.38
22	BA	2748	A	C8-N7	5.14	1.35	1.31
1	AA	373	A	N3-C4	5.14	1.38	1.34
22	BA	1970	A	N7-C5	-5.14	1.36	1.39
22	BA	167	A	N7-C5	-5.14	1.36	1.39
22	BA	497	A	C8-N7	5.14	1.35	1.31
22	BA	2038	G	C6-N1	-5.14	1.35	1.39
22	BA	2075	U	C2-N3	-5.14	1.34	1.37
22	BA	2436	G	C5-C4	-5.14	1.34	1.38
22	BA	2541	A	N9-C8	-5.14	1.33	1.37
22	BA	1980	G	C6-N1	-5.14	1.35	1.39
22	BA	466	A	N9-C8	-5.14	1.33	1.37
22	BA	1603	A	N7-C5	-5.14	1.36	1.39
22	BA	947	A	N9-C8	-5.13	1.33	1.37
22	BA	2821	A	N9-C8	-5.13	1.33	1.37
22	BA	1608	A	N7-C5	-5.13	1.36	1.39
22	BA	23	G	N7-C5	-5.13	1.36	1.39
22	BA	693	A	N7-C5	-5.13	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1154	G	C6-N1	-5.13	1.35	1.39
22	BA	1439	A	N9-C8	-5.13	1.33	1.37
22	BA	1968	G	C8-N7	-5.13	1.27	1.30
22	BA	2758	A	N3-C4	5.13	1.38	1.34
22	BA	799	G	N1-C2	-5.13	1.33	1.37
22	BA	1800	C	N1-C6	-5.13	1.34	1.37
22	BA	2031	A	N7-C5	-5.13	1.36	1.39
22	BA	2070	A	C8-N7	5.13	1.35	1.31
22	BA	2233	U	C2-N3	-5.13	1.34	1.37
22	BA	2376	A	C8-N7	5.13	1.35	1.31
1	AA	49	U	N3-C4	-5.13	1.33	1.38
1	AA	1502	A	C8-N7	5.13	1.35	1.31
22	BA	197	A	N9-C8	-5.13	1.33	1.37
22	BA	727	A	N9-C4	-5.13	1.34	1.37
22	BA	1225	G	C5-C4	-5.13	1.34	1.38
22	BA	1431	A	N9-C8	-5.13	1.33	1.37
22	BA	1992	G	C8-N7	-5.13	1.27	1.30
22	BA	2101	A	N1-C2	5.13	1.39	1.34
22	BA	2252	G	C5-C4	-5.13	1.34	1.38
22	BA	2469	A	N7-C5	-5.13	1.36	1.39
22	BA	2757	A	N3-C4	5.13	1.38	1.34
1	AA	635	A	N3-C4	5.12	1.38	1.34
1	AA	777	A	C8-N7	5.12	1.35	1.31
22	BA	227	A	N7-C5	-5.12	1.36	1.39
22	BA	1212	G	C5-C4	-5.12	1.34	1.38
22	BA	2370	G	N1-C2	-5.12	1.33	1.37
22	BA	2592	G	C6-N1	-5.12	1.35	1.39
23	BB	29	A	N7-C5	-5.12	1.36	1.39
22	BA	19	A	N9-C8	-5.12	1.33	1.37
22	BA	547	A	C2-N3	5.12	1.38	1.33
22	BA	1652	A	N9-C8	-5.12	1.33	1.37
22	BA	2893	A	C8-N7	5.12	1.35	1.31
24	BC	218	PRO	CG-CD	-5.12	1.33	1.50
1	AA	546	A	N3-C4	5.12	1.38	1.34
1	AA	695	A	N3-C4	5.12	1.38	1.34
22	BA	42	A	C8-N7	5.12	1.35	1.31
22	BA	1307	A	N7-C5	-5.12	1.36	1.39
22	BA	2439	A	C8-N7	5.12	1.35	1.31
1	AA	1349	A	N3-C4	5.12	1.38	1.34
22	BA	1371	G	C5-C4	-5.12	1.34	1.38
22	BA	896	A	C2-N3	5.12	1.38	1.33
1	AA	363	A	C8-N7	5.12	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	878	A	N3-C4	5.12	1.38	1.34
22	BA	1663	G	C5-C4	-5.12	1.34	1.38
22	BA	2005	A	N9-C8	-5.12	1.33	1.37
1	AA	1150	A	N3-C4	5.11	1.38	1.34
22	BA	378	C	N3-C4	-5.11	1.30	1.33
22	BA	654	A	C5-C4	-5.11	1.35	1.38
22	BA	928	A	N9-C8	-5.11	1.33	1.37
22	BA	2634	A	N7-C5	-5.11	1.36	1.39
22	BA	739	A	N9-C8	-5.11	1.33	1.37
1	AA	792	A	N9-C8	-5.11	1.33	1.37
1	AA	1534	A	C5-C4	-5.11	1.35	1.38
22	BA	118	A	N7-C5	-5.11	1.36	1.39
22	BA	2434	A	N9-C8	-5.11	1.33	1.37
22	BA	644	A	N9-C8	-5.11	1.33	1.37
22	BA	1796	U	C2-N3	-5.11	1.34	1.37
22	BA	2595	G	C5-C4	-5.11	1.34	1.38
1	AA	873	A	C8-N7	5.11	1.35	1.31
22	BA	682	G	C8-N7	-5.11	1.27	1.30
22	BA	2273	A	N3-C4	5.11	1.38	1.34
22	BA	2722	G	C8-N7	-5.11	1.27	1.30
1	AA	1318	A	N3-C4	5.10	1.38	1.34
22	BA	492	A	N9-C8	-5.10	1.33	1.37
1	AA	539	A	N3-C4	5.10	1.38	1.34
1	AA	629	A	N3-C4	5.10	1.38	1.34
1	AA	1036	A	C5-C4	-5.10	1.35	1.38
22	BA	126	A	N7-C5	-5.10	1.36	1.39
22	BA	1419	A	N3-C4	5.10	1.38	1.34
22	BA	2412	A	N9-C8	-5.10	1.33	1.37
22	BA	1103	A	C5-C4	-5.10	1.35	1.38
22	BA	1312	U	C2-N3	-5.10	1.34	1.37
22	BA	1889	A	C8-N7	5.10	1.35	1.31
22	BA	2038	G	N7-C5	-5.10	1.36	1.39
22	BA	2476	A	N7-C5	-5.10	1.36	1.39
1	AA	1201	A	N1-C2	5.10	1.39	1.34
22	BA	974	G	C6-N1	-5.10	1.35	1.39
22	BA	1634	A	N7-C5	-5.10	1.36	1.39
22	BA	1978	A	N9-C8	-5.10	1.33	1.37
22	BA	2417	C	N3-C4	-5.10	1.30	1.33
22	BA	2543	G	C5-C4	-5.10	1.34	1.38
55	B8	69	A	C5-C4	-5.10	1.35	1.38
22	BA	94	A	N3-C4	5.10	1.38	1.34
22	BA	730	A	N3-C4	5.10	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2620	C	N3-C4	-5.10	1.30	1.33
1	AA	676	A	C8-N7	5.10	1.35	1.31
22	BA	2574	G	C6-N1	-5.10	1.35	1.39
1	AA	1000	A	C2-N3	5.09	1.38	1.33
1	AA	1280	A	N3-C4	5.09	1.38	1.34
22	BA	1246	A	N7-C5	-5.09	1.36	1.39
22	BA	678	C	N3-C4	-5.09	1.30	1.33
22	BA	1801	A	C8-N7	5.09	1.35	1.31
55	B8	26	A	C2-N3	5.09	1.38	1.33
22	BA	126	A	N9-C8	-5.09	1.33	1.37
22	BA	675	A	N9-C8	-5.09	1.33	1.37
22	BA	1151	A	N9-C8	-5.09	1.33	1.37
22	BA	2227	A	N7-C5	-5.09	1.36	1.39
22	BA	2288	A	N9-C8	-5.09	1.33	1.37
22	BA	2516	A	N9-C8	-5.09	1.33	1.37
55	B8	66	A	C5-C4	-5.09	1.35	1.38
1	AA	1176	A	N3-C4	5.09	1.38	1.34
22	BA	182	A	C8-N7	5.09	1.35	1.31
22	BA	849	A	C8-N7	5.09	1.35	1.31
22	BA	207	A	N9-C8	-5.09	1.33	1.37
22	BA	299	A	C8-N7	5.09	1.35	1.31
22	BA	1214	A	N9-C8	-5.09	1.33	1.37
24	BC	247	PRO	CG-CD	-5.09	1.33	1.50
55	B8	69	A	C2-N3	5.09	1.38	1.33
1	AA	190	A	C5-C4	-5.08	1.35	1.38
1	AA	1110	A	N3-C4	5.08	1.37	1.34
22	BA	1901	A	N9-C8	-5.08	1.33	1.37
22	BA	2333	A	C8-N7	5.08	1.35	1.31
22	BA	2686	G	C5-C4	-5.08	1.34	1.38
1	AA	909	A	N7-C5	-5.08	1.36	1.39
22	BA	279	A	N3-C4	5.08	1.37	1.34
22	BA	1701	A	N7-C5	-5.08	1.36	1.39
22	BA	1791	A	N9-C8	-5.08	1.33	1.37
1	AA	640	A	N3-C4	5.08	1.37	1.34
22	BA	1749	A	N7-C5	-5.08	1.36	1.39
22	BA	2879	A	N9-C8	-5.08	1.33	1.37
1	AA	80	A	C5-C4	-5.08	1.35	1.38
1	AA	873	A	N7-C5	-5.08	1.36	1.39
22	BA	1986	C	N3-C4	-5.08	1.30	1.33
22	BA	2635	A	N9-C8	-5.08	1.33	1.37
22	BA	2757	A	C8-N7	5.08	1.35	1.31
23	BB	78	A	C8-N7	5.08	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2530	A	C8-N7	5.08	1.35	1.31
31	BJ	110	PRO	CG-CD	-5.08	1.33	1.50
1	AA	432	A	N3-C4	5.07	1.37	1.34
22	BA	251	A	N9-C8	-5.07	1.33	1.37
22	BA	693	A	N9-C8	-5.07	1.33	1.37
22	BA	1553	A	N7-C5	-5.07	1.36	1.39
22	BA	1927	A	N9-C8	-5.07	1.33	1.37
22	BA	2430	A	N9-C4	-5.07	1.34	1.37
1	AA	44	A	N3-C4	5.07	1.37	1.34
22	BA	415	A	N9-C8	-5.07	1.33	1.37
22	BA	788	A	N7-C5	-5.07	1.36	1.39
22	BA	1054	A	C5-C4	-5.07	1.35	1.38
22	BA	1572	A	N9-C8	-5.07	1.33	1.37
22	BA	2013	A	N9-C8	-5.07	1.33	1.37
22	BA	2027	G	C5-C4	-5.07	1.34	1.38
22	BA	2101	A	C5-C4	-5.07	1.35	1.38
1	AA	807	A	C8-N7	5.07	1.35	1.31
22	BA	636	G	C8-N7	-5.07	1.27	1.30
33	BL	62	PRO	CG-CD	-5.07	1.33	1.50
1	AA	794	A	C8-N7	5.07	1.35	1.31
22	BA	1785	A	N9-C8	-5.07	1.33	1.37
22	BA	2778	A	N7-C5	-5.07	1.36	1.39
22	BA	1285	A	C8-N7	5.07	1.35	1.31
22	BA	1328	A	N9-C8	-5.07	1.33	1.37
25	BD	143	PRO	CG-CD	-5.07	1.33	1.50
22	BA	6	A	C8-N7	5.06	1.35	1.31
22	BA	192	C	C4-C5	-5.06	1.38	1.43
22	BA	809	G	N1-C2	-5.06	1.33	1.37
22	BA	181	A	N7-C5	-5.06	1.36	1.39
22	BA	1477	A	C8-N7	5.06	1.35	1.31
22	BA	2662	A	C8-N7	5.06	1.35	1.31
22	BA	2679	A	N9-C8	-5.06	1.33	1.37
1	AA	1261	A	C5-C4	-5.06	1.35	1.38
22	BA	233	A	N9-C8	-5.06	1.33	1.37
22	BA	820	A	N9-C8	-5.06	1.33	1.37
22	BA	1938	A	C8-N7	5.06	1.35	1.31
22	BA	2068	U	C2-N3	-5.06	1.34	1.37
22	BA	2444	G	N7-C5	-5.06	1.36	1.39
22	BA	2812	G	C6-N1	-5.06	1.36	1.39
1	AA	199	A	N3-C4	5.06	1.37	1.34
22	BA	1794	A	N9-C8	-5.06	1.33	1.37
22	BA	2686	G	N1-C2	-5.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	262	A	N7-C5	-5.06	1.36	1.39
1	AA	1201	A	C2-N3	5.05	1.38	1.33
22	BA	1678	A	C5-C6	-5.05	1.36	1.41
22	BA	217	A	C8-N7	5.05	1.35	1.31
22	BA	1544	A	N7-C5	-5.05	1.36	1.39
22	BA	2183	A	C2-N3	5.05	1.38	1.33
22	BA	1759	A	N9-C8	-5.05	1.33	1.37
22	BA	177	G	N7-C5	-5.05	1.36	1.39
22	BA	2346	A	N7-C5	-5.05	1.36	1.39
23	BB	52	A	C8-N7	5.05	1.35	1.31
1	AA	1271	A	N3-C4	5.05	1.37	1.34
22	BA	584	C	N3-C4	-5.05	1.30	1.33
22	BA	794	A	N7-C5	-5.05	1.36	1.39
22	BA	975	A	N7-C5	-5.05	1.36	1.39
22	BA	1767	G	C5-C4	-5.05	1.34	1.38
24	BC	11	PRO	CG-CD	-5.05	1.33	1.50
48	B0	8	PRO	CG-CD	-5.05	1.33	1.50
22	BA	1274	A	N9-C8	-5.04	1.33	1.37
23	BB	50	A	C8-N7	5.04	1.35	1.31
35	BN	39	PRO	CG-CD	-5.04	1.34	1.50
1	AA	228	A	N3-C4	5.04	1.37	1.34
22	BA	2050	C	N3-C4	-5.04	1.30	1.33
22	BA	2051	A	N9-C8	-5.04	1.33	1.37
1	AA	487	A	N3-C4	5.04	1.37	1.34
1	AA	872	A	N3-C4	5.04	1.37	1.34
22	BA	1947	C	N3-C4	-5.04	1.30	1.33
22	BA	992	C	N3-C4	-5.04	1.30	1.33
22	BA	1620	G	C5-C4	-5.04	1.34	1.38
1	AA	938	A	N3-C4	5.04	1.37	1.34
22	BA	216	A	C8-N7	5.04	1.35	1.31
22	BA	1597	A	N7-C5	-5.04	1.36	1.39
22	BA	2724	U	C2-N3	-5.04	1.34	1.37
24	BC	244	PRO	CG-CD	-5.04	1.34	1.50
1	AA	900	A	N7-C5	-5.04	1.36	1.39
22	BA	2540	C	C2-N3	-5.04	1.31	1.35
22	BA	2823	A	N9-C8	-5.04	1.33	1.37
1	AA	1534	A	N1-C2	5.03	1.38	1.34
22	BA	976	G	C6-N1	-5.03	1.36	1.39
22	BA	2453	A	N9-C8	-5.03	1.33	1.37
22	BA	6	A	N7-C5	-5.03	1.36	1.39
22	BA	2142	A	C2-N3	5.03	1.38	1.33
34	BM	98	PRO	CG-CD	-5.03	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1394	A	N3-C4	5.03	1.37	1.34
22	BA	345	A	N3-C4	5.03	1.37	1.34
22	BA	570	G	C5-C4	-5.03	1.34	1.38
22	BA	1133	A	C8-N7	5.03	1.35	1.31
22	BA	2544	G	C5-C4	-5.03	1.34	1.38
40	BS	87	PRO	CG-CD	-5.03	1.34	1.50
22	BA	1090	A	C2-N3	5.03	1.38	1.33
22	BA	675	A	C5-C6	-5.03	1.36	1.41
22	BA	1050	A	N3-C4	5.03	1.37	1.34
22	BA	1586	A	N3-C4	5.03	1.37	1.34
22	BA	1780	A	N7-C5	-5.03	1.36	1.39
22	BA	1876	A	N3-C4	5.03	1.37	1.34
1	AA	1350	A	N3-C4	5.03	1.37	1.34
22	BA	2258	C	N3-C4	-5.03	1.30	1.33
22	BA	2632	A	C8-N7	5.03	1.35	1.31
22	BA	1667	G	C5-C4	-5.02	1.34	1.38
22	BA	2049	G	C5-C4	-5.02	1.34	1.38
22	BA	911	A	N9-C8	-5.02	1.33	1.37
22	BA	1652	A	N7-C5	-5.02	1.36	1.39
22	BA	2262	U	C2-N3	-5.02	1.34	1.37
22	BA	1899	A	C5-C6	-5.02	1.36	1.41
22	BA	2154	A	C5-C4	-5.02	1.35	1.38
22	BA	2692	G	N7-C5	-5.02	1.36	1.39
45	BX	31	PRO	CG-CD	-5.02	1.34	1.50
1	AA	365	U	C2-N3	-5.02	1.34	1.37
1	AA	794	A	N7-C5	-5.02	1.36	1.39
1	AA	1046	A	C2-N3	5.02	1.38	1.33
22	BA	2126	A	C2-N3	5.02	1.38	1.33
25	BD	205	PRO	CG-CD	-5.02	1.34	1.50
1	AA	1151	A	C2-N3	5.02	1.38	1.33
1	AA	1502	A	N7-C5	-5.02	1.36	1.39
22	BA	1376	C	C4-C5	-5.02	1.39	1.43
22	BA	2176	A	C2-N3	5.02	1.38	1.33
22	BA	2599	G	C6-N1	-5.02	1.36	1.39
25	BD	63	PRO	CG-CD	-5.02	1.34	1.50
55	B8	66	A	C2-N3	5.02	1.38	1.33
22	BA	279	A	C2-N3	5.02	1.38	1.33
22	BA	592	A	N7-C5	-5.02	1.36	1.39
22	BA	962	G	C6-N1	-5.02	1.36	1.39
1	AA	777	A	N7-C5	-5.01	1.36	1.39
22	BA	512	G	C5-C4	-5.01	1.34	1.38
22	BA	590	A	N7-C5	-5.01	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1754	A	N9-C8	-5.01	1.33	1.37
24	BC	32	PRO	CG-CD	-5.01	1.34	1.50
22	BA	1138	G	C8-N7	-5.01	1.27	1.30
1	AA	430	A	C2-N3	5.01	1.38	1.33
1	AA	865	A	N7-C5	-5.01	1.36	1.39
22	BA	244	A	C8-N7	5.01	1.35	1.31
22	BA	322	A	N3-C4	5.01	1.37	1.34
1	AA	98	A	C2-N3	5.01	1.38	1.33
22	BA	504	A	C5-C4	-5.01	1.35	1.38
22	BA	1366	A	N9-C8	-5.01	1.33	1.37
22	BA	1528	A	N7-C5	-5.01	1.36	1.39
22	BA	1957	C	N3-C4	-5.01	1.30	1.33
22	BA	2635	A	N3-C4	5.01	1.37	1.34
22	BA	586	A	C6-N1	-5.01	1.32	1.35
22	BA	971	G	C5-C4	-5.01	1.34	1.38
22	BA	2019	A	N9-C8	-5.01	1.33	1.37
22	BA	2437	G	C6-N1	-5.01	1.36	1.39
1	AA	78	A	C5-C4	-5.00	1.35	1.38
22	BA	959	A	N9-C8	-5.00	1.33	1.37
22	BA	1433	A	C8-N7	5.00	1.35	1.31
22	BA	2369	A	C8-N7	5.00	1.35	1.31
1	AA	782	A	C8-N7	5.00	1.35	1.31
1	AA	1227	A	C5-C4	-5.00	1.35	1.38
22	BA	38	A	C8-N7	5.00	1.35	1.31
22	BA	192	C	N3-C4	-5.00	1.30	1.33
22	BA	423	A	C8-N7	5.00	1.35	1.31
22	BA	583	G	C2-N3	-5.00	1.28	1.32
22	BA	1136	G	C5-C4	-5.00	1.34	1.38
22	BA	1876	A	C2-N3	5.00	1.38	1.33
22	BA	2490	G	C6-N1	-5.00	1.36	1.39
1	AA	1236	A	C2-N3	5.00	1.38	1.33
22	BA	1609	A	N9-C8	-5.00	1.33	1.37
23	BB	94	A	N9-C8	-5.00	1.33	1.37

All (13021) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	752	A	N1-C6-N6	-27.47	102.12	118.60
22	BA	2872	A	N1-C6-N6	-24.44	103.94	118.60
22	BA	1668	A	N1-C6-N6	-24.16	104.11	118.60
22	BA	2062	A	N1-C2-N3	-23.43	117.58	129.30
22	BA	1668	A	N1-C2-N3	-23.24	117.68	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2450	A	N1-C2-N3	-23.15	117.72	129.30
22	BA	514	A	N1-C2-N3	-23.08	117.76	129.30
22	BA	945	A	N1-C6-N6	-22.95	104.83	118.60
22	BA	756	A	N1-C2-N3	-22.87	117.86	129.30
22	BA	1668	A	C2-N3-C4	22.86	122.03	110.60
22	BA	1677	A	N1-C2-N3	-22.79	117.90	129.30
22	BA	1937	A	N1-C6-N6	-22.75	104.95	118.60
22	BA	1354	A	N1-C2-N3	-22.72	117.94	129.30
22	BA	119	A	N1-C2-N3	-22.71	117.94	129.30
22	BA	443	A	N1-C2-N3	-22.68	117.96	129.30
22	BA	2327	A	N1-C6-N6	-22.62	105.03	118.60
22	BA	2766	A	N1-C2-N3	-22.61	117.99	129.30
22	BA	1129	A	N1-C2-N3	-22.57	118.02	129.30
22	BA	1253	A	N1-C2-N3	-22.57	118.02	129.30
22	BA	1204	A	N1-C6-N6	-22.55	105.07	118.60
22	BA	126	A	N1-C6-N6	-22.53	105.08	118.60
23	BB	99	A	N1-C6-N6	-22.44	105.14	118.60
1	AA	101	A	N1-C6-N6	-22.42	105.15	118.60
22	BA	2711	A	N1-C2-N3	-22.41	118.09	129.30
22	BA	466	A	N1-C2-N3	-22.39	118.11	129.30
22	BA	1286	A	N1-C2-N3	-22.36	118.12	129.30
22	BA	2451	A	N1-C6-N6	-22.32	105.21	118.60
22	BA	943	A	N1-C2-N3	-22.26	118.17	129.30
22	BA	2033	A	N1-C6-N6	-22.25	105.25	118.60
54	B7	10	U	O5'-P-OP1	-22.16	84.10	110.70
1	AA	160	A	N1-C6-N6	-22.15	105.31	118.60
22	BA	1970	A	N1-C2-N3	-22.13	118.24	129.30
22	BA	1359	A	N1-C6-N6	-22.10	105.34	118.60
22	BA	299	A	N1-C6-N6	-22.10	105.34	118.60
22	BA	2411	A	N1-C2-N3	-22.09	118.25	129.30
22	BA	2589	A	N1-C2-N3	-22.09	118.25	129.30
1	AA	1035	A	N1-C6-N6	-22.08	105.35	118.60
1	AA	152	A	N1-C6-N6	-22.08	105.35	118.60
22	BA	195	A	N1-C2-N3	-22.07	118.27	129.30
22	BA	2764	A	N1-C6-N6	-22.07	105.36	118.60
1	AA	1035	A	C2-N3-C4	22.03	121.61	110.60
22	BA	972	A	N1-C2-N3	-22.02	118.29	129.30
22	BA	2726	A	N1-C2-N3	-22.01	118.30	129.30
22	BA	84	A	N1-C2-N3	-21.98	118.31	129.30
1	AA	704	A	N1-C2-N3	-21.97	118.31	129.30
22	BA	1133	A	N1-C6-N6	-21.97	105.42	118.60
22	BA	1641	A	N1-C6-N6	-21.96	105.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	538	A	N1-C2-N3	-21.93	118.33	129.30
22	BA	1378	A	N1-C6-N6	-21.92	105.45	118.60
22	BA	213	A	N1-C2-N3	-21.91	118.35	129.30
22	BA	1515	A	N1-C6-N6	-21.91	105.46	118.60
22	BA	53	A	N1-C2-N3	-21.89	118.36	129.30
22	BA	2042	A	N1-C2-N3	-21.89	118.36	129.30
22	BA	1970	A	C2-N3-C4	21.87	121.54	110.60
22	BA	2267	A	C2-N3-C4	21.87	121.54	110.60
1	AA	563	A	N1-C6-N6	-21.84	105.50	118.60
22	BA	1630	A	N1-C6-N6	-21.84	105.50	118.60
22	BA	752	A	C2-N3-C4	21.82	121.51	110.60
22	BA	2542	A	N1-C2-N3	-21.77	118.41	129.30
22	BA	1803	A	N1-C2-N3	-21.77	118.41	129.30
22	BA	825	A	N1-C2-N3	-21.75	118.42	129.30
22	BA	1268	A	N1-C2-N3	-21.75	118.43	129.30
22	BA	503	A	C2-N3-C4	21.73	121.47	110.60
22	BA	2566	A	N1-C2-N3	-21.72	118.44	129.30
22	BA	502	A	C2-N3-C4	21.71	121.46	110.60
22	BA	2518	A	C2-N3-C4	21.71	121.45	110.60
22	BA	2060	A	N1-C2-N3	-21.70	118.45	129.30
22	BA	1419	A	N1-C2-N3	-21.67	118.46	129.30
22	BA	2766	A	C2-N3-C4	21.66	121.43	110.60
22	BA	1253	A	N1-C6-N6	-21.65	105.61	118.60
22	BA	1690	A	N1-C6-N6	-21.63	105.62	118.60
22	BA	195	A	C2-N3-C4	21.63	121.41	110.60
22	BA	309	A	N1-C2-N3	-21.61	118.49	129.30
23	BB	99	A	N1-C2-N3	-21.61	118.50	129.30
1	AA	554	A	N1-C6-N6	-21.61	105.64	118.60
22	BA	2005	A	N1-C2-N3	-21.61	118.50	129.30
1	AA	1179	A	N1-C6-N6	-21.59	105.64	118.60
22	BA	599	A	N1-C2-N3	-21.59	118.51	129.30
22	BA	2682	A	N1-C2-N3	-21.58	118.51	129.30
22	BA	2212	A	N1-C6-N6	-21.58	105.65	118.60
22	BA	38	A	N1-C2-N3	-21.57	118.51	129.30
22	BA	119	A	N1-C6-N6	-21.57	105.66	118.60
22	BA	203	A	N1-C2-N3	-21.54	118.53	129.30
22	BA	1571	A	N1-C2-N3	-21.53	118.53	129.30
22	BA	13	A	C2-N3-C4	21.52	121.36	110.60
22	BA	1264	A	N1-C2-N3	-21.51	118.55	129.30
22	BA	2725	A	N1-C2-N3	-21.51	118.55	129.30
22	BA	833	A	N1-C2-N3	-21.50	118.55	129.30
22	BA	1000	A	N1-C2-N3	-21.48	118.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1805	A	N1-C6-N6	-21.47	105.72	118.60
22	BA	788	A	N1-C2-N3	-21.46	118.57	129.30
22	BA	2829	A	N1-C6-N6	-21.44	105.74	118.60
22	BA	457	A	N1-C6-N6	-21.44	105.74	118.60
22	BA	1570	A	N1-C2-N3	-21.41	118.59	129.30
22	BA	532	A	N1-C2-N3	-21.41	118.59	129.30
22	BA	819	A	C2-N3-C4	21.40	121.30	110.60
22	BA	1431	A	N1-C2-N3	-21.40	118.60	129.30
22	BA	2435	A	N1-C6-N6	-21.39	105.76	118.60
22	BA	2823	A	C2-N3-C4	21.39	121.30	110.60
22	BA	2513	A	N1-C6-N6	-21.38	105.77	118.60
22	BA	526	A	N1-C6-N6	-21.38	105.77	118.60
22	BA	983	A	N1-C2-N3	-21.37	118.61	129.30
22	BA	2051	A	C2-N3-C4	21.37	121.29	110.60
22	BA	2518	A	N1-C2-N3	-21.36	118.62	129.30
22	BA	1247	A	N1-C6-N6	-21.35	105.79	118.60
22	BA	2736	A	N1-C2-N3	-21.35	118.62	129.30
22	BA	2868	A	N1-C2-N3	-21.34	118.63	129.30
22	BA	2451	A	N1-C2-N3	-21.33	118.63	129.30
22	BA	1194	A	N1-C6-N6	-21.33	105.80	118.60
1	AA	16	A	N1-C2-N3	-21.31	118.65	129.30
22	BA	2614	A	C2-N3-C4	21.30	121.25	110.60
23	BB	73	A	N1-C2-N3	-21.30	118.65	129.30
22	BA	199	A	N1-C6-N6	-21.28	105.83	118.60
22	BA	528	A	N1-C6-N6	-21.28	105.83	118.60
22	BA	764	A	N1-C2-N3	-21.27	118.66	129.30
22	BA	196	A	N1-C2-N3	-21.27	118.67	129.30
22	BA	1393	A	N1-C2-N3	-21.24	118.68	129.30
22	BA	53	A	N1-C6-N6	-21.24	105.86	118.60
22	BA	742	A	C2-N3-C4	21.23	121.22	110.60
22	BA	2270	A	N1-C2-N3	-21.23	118.69	129.30
22	BA	670	A	N1-C2-N3	-21.21	118.69	129.30
1	AA	243	A	N1-C6-N6	-21.20	105.88	118.60
1	AA	900	A	C2-N3-C4	21.20	121.20	110.60
22	BA	1342	A	N1-C2-N3	-21.19	118.70	129.30
22	BA	1678	A	N1-C2-N3	-21.17	118.71	129.30
22	BA	1713	A	N1-C6-N6	-21.17	105.90	118.60
22	BA	861	A	N1-C2-N3	-21.17	118.72	129.30
22	BA	2873	A	N1-C2-N3	-21.16	118.72	129.30
22	BA	1759	A	N1-C2-N3	-21.16	118.72	129.30
22	BA	1927	A	N1-C6-N6	-21.14	105.92	118.60
22	BA	2376	A	N1-C2-N3	-21.14	118.73	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	196	A	C2-N3-C4	21.13	121.16	110.60
22	BA	216	A	N1-C2-N3	-21.13	118.74	129.30
22	BA	2883	A	N1-C2-N3	-21.12	118.74	129.30
22	BA	2542	A	C2-N3-C4	21.11	121.16	110.60
22	BA	1610	A	N1-C2-N3	-21.11	118.74	129.30
22	BA	2602	A	N1-C6-N6	-21.11	105.93	118.60
22	BA	819	A	N1-C2-N3	-21.11	118.75	129.30
22	BA	1032	A	N1-C6-N6	-21.10	105.94	118.60
1	AA	1251	A	N1-C6-N6	-21.10	105.94	118.60
55	B8	76	A	N1-C6-N6	-21.09	105.95	118.60
22	BA	1156	A	N1-C2-N3	-21.07	118.76	129.30
22	BA	502	A	N1-C6-N6	-21.06	105.97	118.60
22	BA	1569	A	N1-C2-N3	-21.06	118.77	129.30
22	BA	402	A	N1-C2-N3	-21.05	118.77	129.30
22	BA	2566	A	N1-C6-N6	-21.05	105.97	118.60
22	BA	1626	A	N1-C2-N3	-21.05	118.77	129.30
22	BA	2381	A	N1-C2-N3	-21.05	118.77	129.30
22	BA	2051	A	N1-C2-N3	-21.04	118.78	129.30
22	BA	14	A	N1-C2-N3	-21.03	118.78	129.30
22	BA	38	A	C2-N3-C4	21.03	121.12	110.60
22	BA	2823	A	N1-C6-N6	-21.03	105.98	118.60
22	BA	1028	A	N1-C2-N3	-21.02	118.79	129.30
22	BA	2872	A	N1-C2-N3	-21.02	118.79	129.30
22	BA	984	A	N1-C2-N3	-21.02	118.79	129.30
22	BA	1853	A	N1-C2-N3	-21.02	118.79	129.30
23	BB	99	A	C2-N3-C4	21.01	121.11	110.60
22	BA	2426	A	N1-C2-N3	-21.01	118.80	129.30
1	AA	900	A	N1-C2-N3	-21.00	118.80	129.30
22	BA	1021	A	C2-N3-C4	21.00	121.10	110.60
22	BA	1789	A	N1-C6-N6	-21.00	106.00	118.60
1	AA	675	A	N1-C2-N3	-21.00	118.80	129.30
22	BA	820	A	N1-C2-N3	-20.99	118.81	129.30
22	BA	933	A	N1-C6-N6	-20.99	106.01	118.60
22	BA	1548	A	N1-C2-N3	-20.99	118.81	129.30
1	AA	397	A	C2-N3-C4	20.98	121.09	110.60
22	BA	689	A	N1-C2-N3	-20.98	118.81	129.30
1	AA	71	A	N1-C6-N6	-20.98	106.01	118.60
22	BA	1784	A	N1-C2-N3	-20.98	118.81	129.30
22	BA	1253	A	C2-N3-C4	20.98	121.09	110.60
22	BA	1829	A	C2-N3-C4	20.97	121.08	110.60
22	BA	2665	A	N1-C2-N3	-20.96	118.82	129.30
22	BA	676	A	N1-C2-N3	-20.96	118.82	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1672	A	N1-C2-N3	-20.96	118.82	129.30
22	BA	2033	A	N1-C2-N3	-20.95	118.83	129.30
22	BA	2052	A	C2-N3-C4	20.95	121.08	110.60
22	BA	756	A	C2-N3-C4	20.94	121.07	110.60
22	BA	749	A	N1-C2-N3	-20.93	118.83	129.30
22	BA	750	A	C2-N3-C4	20.93	121.06	110.60
22	BA	608	A	N1-C2-N3	-20.92	118.84	129.30
1	AA	547	A	N1-C6-N6	-20.92	106.05	118.60
22	BA	1129	A	C2-N3-C4	20.91	121.06	110.60
1	AA	1433	A	N1-C2-N3	-20.90	118.85	129.30
22	BA	990	A	N1-C2-N3	-20.89	118.85	129.30
1	AA	977	A	C2-N3-C4	20.89	121.05	110.60
22	BA	1937	A	N1-C2-N3	-20.89	118.85	129.30
22	BA	783	A	C2-N3-C4	20.88	121.04	110.60
22	BA	1189	A	N1-C2-N3	-20.88	118.86	129.30
22	BA	371	A	N1-C6-N6	-20.88	106.07	118.60
22	BA	1287	A	N1-C2-N3	-20.87	118.86	129.30
22	BA	637	A	N1-C2-N3	-20.87	118.87	129.30
22	BA	1354	A	C2-N3-C4	20.87	121.03	110.60
22	BA	631	A	N1-C2-N3	-20.86	118.87	129.30
22	BA	1603	A	N1-C2-N3	-20.86	118.87	129.30
22	BA	2820	A	N1-C2-N3	-20.85	118.87	129.30
22	BA	126	A	N1-C2-N3	-20.85	118.88	129.30
22	BA	764	A	N1-C6-N6	-20.85	106.09	118.60
22	BA	2781	A	N1-C2-N3	-20.85	118.88	129.30
22	BA	1665	A	N1-C2-N3	-20.84	118.88	129.30
22	BA	111	A	N1-C6-N6	-20.84	106.10	118.60
22	BA	2800	A	N1-C6-N6	-20.84	106.10	118.60
22	BA	1635	A	N1-C2-N3	-20.83	118.88	129.30
22	BA	1637	A	N1-C2-N3	-20.83	118.89	129.30
1	AA	465	A	C2-N3-C4	20.82	121.01	110.60
22	BA	1260	A	N1-C2-N3	-20.81	118.89	129.30
1	AA	498	A	C2-N3-C4	20.81	121.00	110.60
22	BA	2009	A	N1-C2-N3	-20.80	118.90	129.30
1	AA	622	A	N1-C6-N6	-20.80	106.12	118.60
22	BA	670	A	C2-N3-C4	20.79	121.00	110.60
22	BA	742	A	N1-C2-N3	-20.79	118.91	129.30
22	BA	330	A	C2-N3-C4	20.79	120.99	110.60
1	AA	563	A	C2-N3-C4	20.78	120.99	110.60
23	BB	58	A	N1-C6-N6	-20.78	106.13	118.60
22	BA	1927	A	N1-C2-N3	-20.78	118.91	129.30
1	AA	621	A	N1-C6-N6	-20.78	106.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	675	A	N1-C2-N3	-20.78	118.91	129.30
22	BA	2542	A	N1-C6-N6	-20.77	106.14	118.60
22	BA	933	A	C2-N3-C4	20.77	120.98	110.60
22	BA	917	A	N1-C2-N3	-20.76	118.92	129.30
22	BA	1328	A	N1-C6-N6	-20.76	106.14	118.60
22	BA	1321	A	N1-C6-N6	-20.76	106.15	118.60
22	BA	2031	A	N1-C2-N3	-20.75	118.92	129.30
22	BA	126	A	C2-N3-C4	20.75	120.97	110.60
22	BA	1665	A	C2-N3-C4	20.74	120.97	110.60
22	BA	1757	A	N1-C2-N3	-20.74	118.93	129.30
22	BA	196	A	N1-C6-N6	-20.74	106.16	118.60
22	BA	89	A	N1-C2-N3	-20.73	118.93	129.30
22	BA	927	A	N1-C2-N3	-20.73	118.93	129.30
1	AA	915	A	N1-C2-N3	-20.73	118.93	129.30
22	BA	1772	A	N1-C2-N3	-20.73	118.94	129.30
22	BA	825	A	C2-N3-C4	20.73	120.96	110.60
22	BA	2765	A	C2-N3-C4	20.72	120.96	110.60
22	BA	1009	A	N1-C2-N3	-20.72	118.94	129.30
22	BA	750	A	N1-C2-N3	-20.72	118.94	129.30
22	BA	1932	A	N1-C2-N3	-20.72	118.94	129.30
22	BA	457	A	N1-C2-N3	-20.72	118.94	129.30
22	BA	1937	A	C2-N3-C4	20.71	120.96	110.60
22	BA	457	A	C2-N3-C4	20.71	120.95	110.60
22	BA	582	A	N1-C2-N3	-20.70	118.95	129.30
1	AA	1476	A	N1-C2-N3	-20.70	118.95	129.30
22	BA	1650	A	N1-C2-N3	-20.69	118.95	129.30
22	BA	2635	A	C2-N3-C4	20.69	120.95	110.60
22	BA	910	A	N1-C2-N3	-20.69	118.95	129.30
22	BA	941	A	N1-C2-N3	-20.69	118.95	129.30
22	BA	2062	A	N1-C6-N6	-20.69	106.19	118.60
1	AA	26	A	N1-C2-N3	-20.68	118.96	129.30
1	AA	1428	A	N1-C6-N6	-20.68	106.19	118.60
22	BA	74	A	N1-C6-N6	-20.68	106.19	118.60
22	BA	1156	A	C2-N3-C4	20.68	120.94	110.60
1	AA	621	A	C2-N3-C4	20.67	120.94	110.60
1	AA	792	A	C2-N3-C4	20.67	120.93	110.60
22	BA	621	A	N1-C2-N3	-20.66	118.97	129.30
1	AA	195	A	N1-C2-N3	-20.66	118.97	129.30
22	BA	2589	A	C2-N3-C4	20.66	120.93	110.60
22	BA	917	A	C2-N3-C4	20.65	120.93	110.60
22	BA	960	A	C2-N3-C4	20.65	120.93	110.60
22	BA	466	A	C2-N3-C4	20.65	120.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2823	A	N1-C2-N3	-20.65	118.98	129.30
22	BA	1262	A	N1-C2-N3	-20.65	118.98	129.30
22	BA	217	A	N1-C2-N3	-20.64	118.98	129.30
1	AA	918	A	N1-C6-N6	-20.64	106.22	118.60
1	AA	729	A	N1-C6-N6	-20.63	106.22	118.60
1	AA	1333	A	N1-C6-N6	-20.63	106.22	118.60
22	BA	821	A	N1-C6-N6	-20.62	106.23	118.60
23	BB	101	A	C2-N3-C4	20.62	120.91	110.60
22	BA	933	A	N1-C2-N3	-20.62	118.99	129.30
22	BA	1001	A	N1-C6-N6	-20.62	106.23	118.60
22	BA	1392	A	C2-N3-C4	20.62	120.91	110.60
1	AA	1016	A	N1-C6-N6	-20.62	106.23	118.60
22	BA	2005	A	C2-N3-C4	20.62	120.91	110.60
22	BA	1142	A	N1-C6-N6	-20.62	106.23	118.60
22	BA	802	A	N1-C6-N6	-20.61	106.23	118.60
1	AA	363	A	C2-N3-C4	20.60	120.90	110.60
22	BA	2887	A	N1-C2-N3	-20.60	119.00	129.30
22	BA	730	A	N1-C2-N3	-20.60	119.00	129.30
22	BA	2003	A	N1-C2-N3	-20.60	119.00	129.30
22	BA	2070	A	C2-N3-C4	20.60	120.90	110.60
22	BA	2736	A	C2-N3-C4	20.59	120.90	110.60
22	BA	222	A	N1-C2-N3	-20.59	119.00	129.30
1	AA	81	A	N1-C6-N6	-20.59	106.25	118.60
22	BA	1570	A	C2-N3-C4	20.59	120.90	110.60
22	BA	310	A	N1-C2-N3	-20.59	119.01	129.30
22	BA	423	A	N1-C2-N3	-20.58	119.01	129.30
1	AA	622	A	N1-C2-N3	-20.58	119.01	129.30
22	BA	309	A	C2-N3-C4	20.58	120.89	110.60
22	BA	453	A	N1-C2-N3	-20.57	119.01	129.30
22	BA	522	A	C2-N3-C4	20.57	120.89	110.60
22	BA	2883	A	N1-C6-N6	-20.57	106.25	118.60
22	BA	2247	A	N1-C2-N3	-20.57	119.01	129.30
22	BA	1966	A	N1-C6-N6	-20.57	106.26	118.60
22	BA	2657	A	N1-C2-N3	-20.57	119.01	129.30
22	BA	2835	A	N1-C6-N6	-20.57	106.26	118.60
22	BA	1392	A	N1-C2-N3	-20.57	119.02	129.30
23	BB	101	A	N1-C6-N6	-20.56	106.26	118.60
22	BA	1308	A	N1-C6-N6	-20.56	106.27	118.60
1	AA	777	A	N1-C6-N6	-20.55	106.27	118.60
22	BA	1213	A	N1-C2-N3	-20.55	119.02	129.30
22	BA	320	A	N1-C2-N3	-20.55	119.02	129.30
1	AA	461	A	N1-C6-N6	-20.55	106.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	231	A	C2-N3-C4	20.55	120.88	110.60
22	BA	1214	A	N1-C2-N3	-20.55	119.03	129.30
22	BA	1327	A	N1-C2-N3	-20.55	119.03	129.30
22	BA	2632	A	N1-C6-N6	-20.55	106.27	118.60
22	BA	1597	A	C2-N3-C4	20.54	120.87	110.60
22	BA	2270	A	C2-N3-C4	20.54	120.87	110.60
22	BA	502	A	N1-C2-N3	-20.53	119.03	129.30
22	BA	2434	A	N1-C6-N6	-20.52	106.28	118.60
22	BA	984	A	N1-C6-N6	-20.52	106.29	118.60
1	AA	759	A	N1-C6-N6	-20.51	106.29	118.60
22	BA	1039	A	N1-C2-N3	-20.51	119.05	129.30
22	BA	2809	A	N1-C2-N3	-20.51	119.05	129.30
22	BA	199	A	N1-C2-N3	-20.51	119.05	129.30
22	BA	2476	A	N1-C2-N3	-20.50	119.05	129.30
22	BA	602	A	N1-C2-N3	-20.50	119.05	129.30
1	AA	306	A	N1-C2-N3	-20.49	119.05	129.30
22	BA	56	A	N1-C2-N3	-20.49	119.05	129.30
22	BA	743	A	C2-N3-C4	20.49	120.85	110.60
22	BA	800	A	N1-C2-N3	-20.49	119.06	129.30
1	AA	1433	A	C2-N3-C4	20.49	120.84	110.60
22	BA	244	A	N1-C6-N6	-20.48	106.31	118.60
1	AA	282	A	N1-C2-N3	-20.48	119.06	129.30
22	BA	2600	A	N1-C2-N3	-20.48	119.06	129.30
22	BA	412	A	N1-C2-N3	-20.48	119.06	129.30
22	BA	14	A	N1-C6-N6	-20.48	106.31	118.60
22	BA	2635	A	N1-C6-N6	-20.47	106.32	118.60
22	BA	1151	A	C2-N3-C4	20.46	120.83	110.60
22	BA	1427	A	N1-C2-N3	-20.46	119.07	129.30
22	BA	689	A	C2-N3-C4	20.46	120.83	110.60
22	BA	2381	A	N1-C6-N6	-20.45	106.33	118.60
1	AA	243	A	N1-C2-N3	-20.45	119.07	129.30
22	BA	1165	A	N1-C2-N3	-20.45	119.07	129.30
22	BA	1285	A	N1-C2-N3	-20.45	119.08	129.30
22	BA	1783	A	N1-C2-N3	-20.45	119.08	129.30
22	BA	2080	A	N1-C2-N3	-20.45	119.08	129.30
22	BA	1978	A	N1-C2-N3	-20.44	119.08	129.30
22	BA	1134	A	C2-N3-C4	20.44	120.82	110.60
22	BA	2071	A	N1-C2-N3	-20.44	119.08	129.30
22	BA	2418	A	N1-C2-N3	-20.44	119.08	129.30
22	BA	1652	A	N1-C2-N3	-20.44	119.08	129.30
22	BA	2119	A	N1-C6-N6	-20.43	106.34	118.60
22	BA	2748	A	N1-C2-N3	-20.43	119.08	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	74	A	N1-C2-N3	-20.43	119.09	129.30
1	AA	716	A	C2-N3-C4	20.43	120.81	110.60
22	BA	2013	A	N1-C2-N3	-20.43	119.09	129.30
1	AA	1167	A	N1-C6-N6	-20.43	106.34	118.60
22	BA	1701	A	N1-C2-N3	-20.42	119.09	129.30
22	BA	2448	A	N1-C6-N6	-20.42	106.35	118.60
22	BA	2635	A	N1-C2-N3	-20.42	119.09	129.30
1	AA	119	A	N1-C6-N6	-20.41	106.35	118.60
22	BA	1936	A	C2-N3-C4	20.41	120.81	110.60
1	AA	807	A	N1-C6-N6	-20.41	106.35	118.60
1	AA	1035	A	N1-C2-N3	-20.41	119.09	129.30
1	AA	431	A	N1-C6-N6	-20.41	106.35	118.60
22	BA	1155	A	N1-C6-N6	-20.40	106.36	118.60
22	BA	2077	A	N1-C2-N3	-20.39	119.10	129.30
22	BA	2764	A	C2-N3-C4	20.39	120.80	110.60
1	AA	1213	A	N1-C2-N3	-20.39	119.10	129.30
22	BA	299	A	C2-N3-C4	20.39	120.80	110.60
22	BA	2821	A	N1-C2-N3	-20.39	119.10	129.30
22	BA	2225	A	N1-C2-N3	-20.39	119.10	129.30
22	BA	1175	A	C2-N3-C4	20.39	120.79	110.60
1	AA	845	A	N1-C6-N6	-20.38	106.37	118.60
22	BA	670	A	N1-C6-N6	-20.38	106.37	118.60
22	BA	1593	A	N1-C2-N3	-20.38	119.11	129.30
22	BA	1705	A	N1-C2-N3	-20.37	119.11	129.30
22	BA	1640	A	N1-C2-N3	-20.37	119.11	129.30
1	AA	766	A	N1-C2-N3	-20.37	119.11	129.30
1	AA	1213	A	N1-C6-N6	-20.37	106.38	118.60
22	BA	1385	A	N1-C6-N6	-20.37	106.38	118.60
22	BA	1815	A	N1-C2-N3	-20.37	119.12	129.30
22	BA	119	A	C2-N3-C4	20.37	120.78	110.60
22	BA	1262	A	C2-N3-C4	20.36	120.78	110.60
22	BA	2267	A	N1-C6-N6	-20.35	106.39	118.60
22	BA	920	A	N1-C2-N3	-20.35	119.12	129.30
22	BA	1419	A	N1-C6-N6	-20.35	106.39	118.60
22	BA	222	A	C2-N3-C4	20.35	120.77	110.60
1	AA	695	A	N1-C2-N3	-20.35	119.13	129.30
22	BA	1385	A	N1-C2-N3	-20.34	119.13	129.30
1	AA	8	A	N1-C2-N3	-20.34	119.13	129.30
22	BA	792	A	N1-C2-N3	-20.34	119.13	129.30
22	BA	1598	A	N1-C6-N6	-20.33	106.40	118.60
22	BA	2070	A	N1-C6-N6	-20.33	106.40	118.60
22	BA	422	A	N1-C2-N3	-20.32	119.14	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2241	A	N1-C2-N3	-20.32	119.14	129.30
22	BA	960	A	N1-C6-N6	-20.32	106.41	118.60
1	AA	1413	A	N1-C2-N3	-20.32	119.14	129.30
22	BA	330	A	N1-C2-N3	-20.32	119.14	129.30
22	BA	1431	A	C2-N3-C4	20.31	120.76	110.60
22	BA	2639	A	N1-C2-N3	-20.31	119.14	129.30
1	AA	759	A	N1-C2-N3	-20.31	119.14	129.30
22	BA	532	A	C2-N3-C4	20.31	120.75	110.60
22	BA	1932	A	N1-C6-N6	-20.31	106.41	118.60
22	BA	2435	A	N1-C2-N3	-20.31	119.14	129.30
22	BA	2468	A	N1-C2-N3	-20.31	119.15	129.30
22	BA	1111	A	N1-C2-N3	-20.30	119.15	129.30
22	BA	1354	A	N1-C6-N6	-20.30	106.42	118.60
1	AA	1285	A	N1-C2-N3	-20.30	119.15	129.30
22	BA	1701	A	N1-C6-N6	-20.30	106.42	118.60
22	BA	2572	A	N1-C6-N6	-20.30	106.42	118.60
22	BA	160	A	N1-C2-N3	-20.30	119.15	129.30
22	BA	2227	A	N1-C2-N3	-20.29	119.15	129.30
22	BA	2753	A	N1-C2-N3	-20.29	119.15	129.30
1	AA	71	A	N1-C2-N3	-20.27	119.16	129.30
22	BA	1809	A	C2-N3-C4	20.27	120.74	110.60
22	BA	699	A	N1-C2-N3	-20.27	119.17	129.30
22	BA	1285	A	N1-C6-N6	-20.26	106.44	118.60
22	BA	975	A	N1-C2-N3	-20.26	119.17	129.30
22	BA	1809	A	N1-C2-N3	-20.26	119.17	129.30
22	BA	1785	A	N1-C6-N6	-20.26	106.44	118.60
22	BA	2469	A	N1-C2-N3	-20.26	119.17	129.30
22	BA	792	A	C2-N3-C4	20.25	120.73	110.60
22	BA	959	A	N1-C2-N3	-20.25	119.17	129.30
22	BA	1665	A	N1-C6-N6	-20.25	106.45	118.60
22	BA	1274	A	N1-C2-N3	-20.25	119.18	129.30
22	BA	2856	A	N1-C2-N3	-20.25	119.18	129.30
22	BA	825	A	N1-C6-N6	-20.25	106.45	118.60
22	BA	1419	A	C2-N3-C4	20.25	120.72	110.60
22	BA	575	A	N1-C2-N3	-20.24	119.18	129.30
22	BA	1226	A	N1-C2-N3	-20.24	119.18	129.30
22	BA	2776	A	N1-C6-N6	-20.24	106.45	118.60
1	AA	461	A	N1-C2-N3	-20.24	119.18	129.30
22	BA	1194	A	N1-C2-N3	-20.24	119.18	129.30
22	BA	804	A	N1-C2-N3	-20.23	119.18	129.30
22	BA	1650	A	N1-C6-N6	-20.23	106.46	118.60
22	BA	918	A	N1-C2-N3	-20.23	119.19	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2665	A	C2-N3-C4	20.23	120.72	110.60
1	AA	816	A	N1-C2-N3	-20.23	119.19	129.30
22	BA	332	A	N1-C6-N6	-20.23	106.46	118.60
22	BA	1705	A	C2-N3-C4	20.23	120.71	110.60
1	AA	977	A	N1-C6-N6	-20.22	106.47	118.60
22	BA	984	A	C2-N3-C4	20.22	120.71	110.60
22	BA	1008	A	N1-C2-N3	-20.22	119.19	129.30
22	BA	1322	A	N1-C2-N3	-20.22	119.19	129.30
22	BA	1927	A	C2-N3-C4	20.22	120.71	110.60
22	BA	1165	A	N1-C6-N6	-20.21	106.47	118.60
22	BA	1384	A	N1-C2-N3	-20.21	119.19	129.30
1	AA	50	A	C2-N3-C4	20.21	120.71	110.60
22	BA	2639	A	C2-N3-C4	20.21	120.71	110.60
22	BA	515	A	N1-C2-N3	-20.21	119.19	129.30
22	BA	1144	A	N1-C2-N3	-20.21	119.19	129.30
1	AA	1446	A	N1-C6-N6	-20.21	106.47	118.60
22	BA	821	A	N1-C2-N3	-20.21	119.19	129.30
1	AA	704	A	C2-N3-C4	20.21	120.70	110.60
22	BA	1535	A	C2-N3-C4	20.20	120.70	110.60
1	AA	792	A	N1-C2-N3	-20.20	119.20	129.30
22	BA	2369	A	N1-C2-N3	-20.20	119.20	129.30
1	AA	195	A	C2-N3-C4	20.19	120.70	110.60
1	AA	1246	A	C2-N3-C4	20.19	120.70	110.60
22	BA	1133	A	C2-N3-C4	20.19	120.70	110.60
22	BA	2675	A	C2-N3-C4	20.19	120.70	110.60
22	BA	2020	A	N1-C2-N3	-20.19	119.20	129.30
22	BA	2632	A	N1-C2-N3	-20.19	119.20	129.30
22	BA	2766	A	N1-C6-N6	-20.19	106.49	118.60
22	BA	6	A	N1-C6-N6	-20.18	106.49	118.60
22	BA	2434	A	C2-N3-C4	20.18	120.69	110.60
1	AA	607	A	N1-C6-N6	-20.18	106.49	118.60
1	AA	327	A	N1-C2-N3	-20.18	119.21	129.30
22	BA	685	A	C2-N3-C4	20.18	120.69	110.60
22	BA	2758	A	N1-C2-N3	-20.18	119.21	129.30
1	AA	1362	A	N1-C6-N6	-20.18	106.50	118.60
22	BA	538	A	C2-N3-C4	20.17	120.69	110.60
22	BA	1274	A	C2-N3-C4	20.17	120.69	110.60
22	BA	49	A	N1-C2-N3	-20.17	119.22	129.30
22	BA	1762	A	N1-C6-N6	-20.16	106.50	118.60
22	BA	2577	A	N1-C2-N3	-20.16	119.22	129.30
1	AA	50	A	N1-C2-N3	-20.16	119.22	129.30
22	BA	2281	A	N1-C2-N3	-20.16	119.22	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2590	A	N1-C2-N3	-20.16	119.22	129.30
22	BA	432	A	N1-C2-N3	-20.15	119.22	129.30
22	BA	1789	A	C2-N3-C4	20.15	120.67	110.60
1	AA	1289	A	N1-C6-N6	-20.14	106.52	118.60
22	BA	412	A	C2-N3-C4	20.14	120.67	110.60
22	BA	1711	A	N1-C2-N3	-20.14	119.23	129.30
22	BA	1610	A	C2-N3-C4	20.13	120.67	110.60
22	BA	2564	A	N1-C6-N6	-20.13	106.52	118.60
22	BA	693	A	C2-N3-C4	20.13	120.67	110.60
22	BA	56	A	C2-N3-C4	20.13	120.66	110.60
22	BA	1987	A	N1-C2-N3	-20.13	119.23	129.30
22	BA	2358	A	N1-C2-N3	-20.13	119.23	129.30
1	AA	969	A	N1-C2-N3	-20.13	119.24	129.30
22	BA	310	A	C2-N3-C4	20.13	120.66	110.60
22	BA	2868	A	C2-N3-C4	20.12	120.66	110.60
1	AA	607	A	N1-C2-N3	-20.12	119.24	129.30
22	BA	1308	A	N1-C2-N3	-20.12	119.24	129.30
1	AA	572	A	N1-C6-N6	-20.11	106.53	118.60
22	BA	1111	A	C2-N3-C4	20.11	120.66	110.60
22	BA	1308	A	C2-N3-C4	20.11	120.66	110.60
22	BA	877	A	C2-N3-C4	20.11	120.66	110.60
22	BA	1126	A	N1-C6-N6	-20.11	106.53	118.60
22	BA	182	A	N1-C6-N6	-20.11	106.54	118.60
22	BA	1919	A	N1-C2-N3	-20.11	119.25	129.30
1	AA	1022	A	N1-C2-N3	-20.11	119.25	129.30
22	BA	1652	A	N1-C6-N6	-20.11	106.54	118.60
22	BA	1151	A	N1-C2-N3	-20.10	119.25	129.30
22	BA	1637	A	C2-N3-C4	20.10	120.65	110.60
22	BA	371	A	N1-C2-N3	-20.10	119.25	129.30
1	AA	282	A	C2-N3-C4	20.10	120.65	110.60
22	BA	460	A	N1-C2-N3	-20.10	119.25	129.30
22	BA	503	A	N1-C2-N3	-20.09	119.25	129.30
1	AA	1246	A	N1-C6-N6	-20.09	106.54	118.60
22	BA	2070	A	N1-C2-N3	-20.09	119.25	129.30
1	AA	1357	A	C2-N3-C4	20.09	120.64	110.60
22	BA	401	A	N1-C2-N3	-20.09	119.26	129.30
22	BA	734	A	N1-C2-N3	-20.08	119.26	129.30
22	BA	1000	A	C2-N3-C4	20.08	120.64	110.60
22	BA	743	A	N1-C2-N3	-20.08	119.26	129.30
22	BA	2173	A	N1-C6-N6	-20.08	106.55	118.60
22	BA	1535	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	802	A	C2-N3-C4	20.07	120.63	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2392	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	1583	A	N1-C2-N3	-20.07	119.27	129.30
1	AA	374	A	C2-N3-C4	20.06	120.63	110.60
22	BA	504	A	C2-N3-C4	20.06	120.63	110.60
22	BA	2761	A	C2-N3-C4	20.06	120.63	110.60
22	BA	529	A	N1-C6-N6	-20.06	106.56	118.60
22	BA	792	A	N1-C6-N6	-20.06	106.57	118.60
22	BA	2058	A	N1-C2-N3	-20.05	119.27	129.30
1	AA	1171	A	C2-N3-C4	20.05	120.63	110.60
1	AA	802	A	N1-C2-N3	-20.05	119.28	129.30
22	BA	1544	A	C2-N3-C4	20.05	120.62	110.60
1	AA	889	A	N1-C6-N6	-20.05	106.57	118.60
22	BA	1998	A	C2-N3-C4	20.05	120.62	110.60
1	AA	174	A	N1-C6-N6	-20.04	106.57	118.60
22	BA	1819	A	C2-N3-C4	20.04	120.62	110.60
22	BA	262	A	N1-C6-N6	-20.04	106.57	118.60
22	BA	2726	A	C2-N3-C4	20.04	120.62	110.60
22	BA	2288	A	N1-C2-N3	-20.04	119.28	129.30
22	BA	1254	A	N1-C2-N3	-20.04	119.28	129.30
22	BA	1805	A	C2-N3-C4	20.04	120.62	110.60
22	BA	213	A	C2-N3-C4	20.04	120.62	110.60
22	BA	1571	A	C2-N3-C4	20.03	120.61	110.60
22	BA	2879	A	C2-N3-C4	20.03	120.61	110.60
1	AA	977	A	N1-C2-N3	-20.02	119.29	129.30
22	BA	1001	A	N1-C2-N3	-20.02	119.29	129.30
1	AA	665	A	N1-C2-N3	-20.02	119.29	129.30
22	BA	2882	A	N1-C6-N6	-20.02	106.59	118.60
22	BA	556	A	N1-C2-N3	-20.02	119.29	129.30
22	BA	1321	A	C2-N3-C4	20.01	120.61	110.60
22	BA	1027	A	N1-C2-N3	-20.00	119.30	129.30
22	BA	1786	A	C2-N3-C4	20.00	120.60	110.60
1	AA	767	A	N1-C2-N3	-20.00	119.30	129.30
22	BA	1608	A	N1-C2-N3	-20.00	119.30	129.30
22	BA	599	A	C2-N3-C4	20.00	120.60	110.60
22	BA	501	A	N1-C2-N3	-19.99	119.30	129.30
22	BA	152	A	N1-C2-N3	-19.99	119.31	129.30
22	BA	428	A	N1-C2-N3	-19.99	119.31	129.30
22	BA	1262	A	N1-C6-N6	-19.99	106.61	118.60
1	AA	1500	A	C2-N3-C4	19.98	120.59	110.60
22	BA	2031	A	C2-N3-C4	19.98	120.59	110.60
22	BA	1366	A	N1-C2-N3	-19.98	119.31	129.30
22	BA	2406	A	N1-C2-N3	-19.98	119.31	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2753	A	N1-C6-N6	-19.98	106.61	118.60
22	BA	1754	A	N1-C2-N3	-19.97	119.31	129.30
22	BA	111	A	N1-C2-N3	-19.97	119.31	129.30
22	BA	845	A	C2-N3-C4	19.97	120.58	110.60
22	BA	199	A	C2-N3-C4	19.97	120.58	110.60
22	BA	1147	A	C2-N3-C4	19.96	120.58	110.60
22	BA	1876	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	2126	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	1998	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	2080	A	C2-N3-C4	19.96	120.58	110.60
22	BA	207	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	2267	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	1772	A	N1-C6-N6	-19.96	106.63	118.60
22	BA	2094	A	N1-C2-N3	-19.95	119.32	129.30
22	BA	2158	A	N1-C6-N6	-19.95	106.63	118.60
22	BA	1978	A	C2-N3-C4	19.95	120.58	110.60
22	BA	497	A	N1-C2-N3	-19.95	119.32	129.30
22	BA	917	A	N1-C6-N6	-19.95	106.63	118.60
1	AA	753	A	N1-C6-N6	-19.95	106.63	118.60
1	AA	1101	A	N1-C6-N6	-19.95	106.63	118.60
22	BA	1420	A	N1-C2-N3	-19.95	119.33	129.30
22	BA	1566	A	N1-C2-N3	-19.95	119.33	129.30
22	BA	1821	A	N1-C6-N6	-19.95	106.63	118.60
22	BA	64	A	C2-N3-C4	19.94	120.57	110.60
22	BA	1244	A	N1-C2-N3	-19.94	119.33	129.30
1	AA	77	A	N1-C2-N3	-19.94	119.33	129.30
1	AA	303	A	N1-C2-N3	-19.94	119.33	129.30
22	BA	241	A	N1-C2-N3	-19.94	119.33	129.30
22	BA	833	A	C2-N3-C4	19.94	120.57	110.60
22	BA	1854	A	N1-C2-N3	-19.94	119.33	129.30
22	BA	2577	A	C2-N3-C4	19.94	120.57	110.60
22	BA	2327	A	C2-N3-C4	19.94	120.57	110.60
22	BA	2476	A	C2-N3-C4	19.94	120.57	110.60
1	AA	306	A	C2-N3-C4	19.93	120.57	110.60
1	AA	373	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	1664	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	1966	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	1640	A	N1-C6-N6	-19.93	106.64	118.60
1	AA	393	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	2273	A	C2-N3-C4	19.93	120.57	110.60
22	BA	216	A	N1-C6-N6	-19.93	106.64	118.60
22	BA	2058	A	N1-C6-N6	-19.93	106.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2856	A	C2-N3-C4	19.93	120.56	110.60
22	BA	2266	A	N1-C2-N3	-19.93	119.34	129.30
1	AA	790	A	N1-C2-N3	-19.93	119.34	129.30
1	AA	1180	A	N1-C2-N3	-19.93	119.34	129.30
22	BA	1759	A	C2-N3-C4	19.92	120.56	110.60
22	BA	1762	A	N1-C2-N3	-19.92	119.34	129.30
22	BA	1932	A	C2-N3-C4	19.92	120.56	110.60
22	BA	477	A	N1-C2-N3	-19.92	119.34	129.30
22	BA	2158	A	C2-N3-C4	19.92	120.56	110.60
1	AA	520	A	N1-C6-N6	-19.92	106.65	118.60
22	BA	2033	A	C2-N3-C4	19.92	120.56	110.60
22	BA	345	A	C2-N3-C4	19.91	120.56	110.60
22	BA	789	A	N1-C2-N3	-19.91	119.34	129.30
22	BA	2411	A	C2-N3-C4	19.91	120.56	110.60
1	AA	694	A	N1-C2-N3	-19.91	119.35	129.30
22	BA	2346	A	N1-C6-N6	-19.91	106.66	118.60
22	BA	412	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	699	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	739	A	N1-C2-N3	-19.90	119.35	129.30
22	BA	74	A	C2-N3-C4	19.90	120.55	110.60
1	AA	547	A	C2-N3-C4	19.90	120.55	110.60
1	AA	787	A	N1-C6-N6	-19.90	106.66	118.60
1	AA	1157	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	190	A	N1-C2-N3	-19.89	119.35	129.30
22	BA	2749	A	N1-C6-N6	-19.89	106.66	118.60
22	BA	2837	A	N1-C2-N3	-19.89	119.35	129.30
22	BA	1469	A	N1-C2-N3	-19.89	119.35	129.30
23	BB	52	A	N1-C2-N3	-19.89	119.35	129.30
22	BA	241	A	C2-N3-C4	19.89	120.55	110.60
22	BA	514	A	C2-N3-C4	19.89	120.54	110.60
22	BA	1641	A	N1-C2-N3	-19.89	119.36	129.30
22	BA	2297	A	N1-C6-N6	-19.89	106.67	118.60
1	AA	546	A	N1-C2-N3	-19.88	119.36	129.30
22	BA	2270	A	N1-C6-N6	-19.88	106.67	118.60
1	AA	197	A	N1-C2-N3	-19.88	119.36	129.30
22	BA	449	A	C2-N3-C4	19.88	120.54	110.60
22	BA	586	A	N1-C6-N6	-19.88	106.67	118.60
22	BA	1189	A	C2-N3-C4	19.88	120.54	110.60
1	AA	1042	A	N1-C6-N6	-19.88	106.67	118.60
22	BA	2135	A	C2-N3-C4	19.88	120.54	110.60
22	BA	1525	A	N1-C6-N6	-19.87	106.68	118.60
22	BA	2406	A	N1-C6-N6	-19.87	106.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2547	A	N1-C2-N3	-19.87	119.36	129.30
22	BA	2778	A	N1-C6-N6	-19.87	106.68	118.60
1	AA	919	A	N1-C6-N6	-19.87	106.68	118.60
22	BA	479	A	N1-C2-N3	-19.87	119.36	129.30
22	BA	1495	A	N1-C2-N3	-19.87	119.36	129.30
22	BA	223	A	N1-C2-N3	-19.87	119.37	129.30
22	BA	1403	A	N1-C6-N6	-19.87	106.68	118.60
1	AA	621	A	N1-C2-N3	-19.87	119.37	129.30
22	BA	384	A	N1-C2-N3	-19.87	119.37	129.30
22	BA	1900	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	244	A	N1-C2-N3	-19.86	119.37	129.30
1	AA	959	A	C2-N3-C4	19.86	120.53	110.60
22	BA	404	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	1572	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	2278	A	N1-C6-N6	-19.86	106.69	118.60
22	BA	1395	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	1021	A	N1-C6-N6	-19.86	106.69	118.60
22	BA	2587	A	N1-C2-N3	-19.85	119.37	129.30
22	BA	2826	A	N1-C2-N3	-19.85	119.37	129.30
1	AA	411	A	N1-C2-N3	-19.85	119.37	129.30
1	AA	131	A	N1-C2-N3	-19.85	119.37	129.30
22	BA	1244	A	N1-C6-N6	-19.85	106.69	118.60
1	AA	274	A	N1-C2-N3	-19.85	119.38	129.30
1	AA	825	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	1544	A	N1-C2-N3	-19.85	119.38	129.30
22	BA	2077	A	C2-N3-C4	19.84	120.52	110.60
22	BA	928	A	N1-C2-N3	-19.84	119.38	129.30
22	BA	1142	A	C2-N3-C4	19.84	120.52	110.60
22	BA	1067	A	N1-C2-N3	-19.84	119.38	129.30
22	BA	1553	A	N1-C2-N3	-19.84	119.38	129.30
1	AA	872	A	N1-C2-N3	-19.83	119.38	129.30
22	BA	1936	A	N1-C2-N3	-19.83	119.38	129.30
22	BA	2369	A	C2-N3-C4	19.83	120.52	110.60
1	AA	780	A	N1-C2-N3	-19.83	119.39	129.30
1	AA	10	A	N1-C2-N3	-19.83	119.39	129.30
22	BA	2675	A	N1-C2-N3	-19.83	119.39	129.30
22	BA	2810	A	N1-C2-N3	-19.83	119.39	129.30
22	BA	439	A	C2-N3-C4	19.82	120.51	110.60
22	BA	270	A	N1-C2-N3	-19.82	119.39	129.30
22	BA	1095	A	C2-N3-C4	19.82	120.51	110.60
22	BA	1470	A	N1-C2-N3	-19.82	119.39	129.30
22	BA	1365	A	C2-N3-C4	19.82	120.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	637	A	C2-N3-C4	19.81	120.51	110.60
22	BA	693	A	N1-C6-N6	-19.81	106.71	118.60
22	BA	1515	A	C2-N3-C4	19.81	120.51	110.60
1	AA	181	A	N1-C2-N3	-19.81	119.39	129.30
1	AA	1465	A	N1-C6-N6	-19.81	106.72	118.60
22	BA	972	A	C2-N3-C4	19.81	120.50	110.60
1	AA	139	A	C2-N3-C4	19.81	120.50	110.60
22	BA	508	A	C2-N3-C4	19.81	120.50	110.60
22	BA	1916	A	N1-C6-N6	-19.81	106.72	118.60
1	AA	900	A	N1-C6-N6	-19.80	106.72	118.60
22	BA	423	A	N1-C6-N6	-19.80	106.72	118.60
22	BA	1591	A	C2-N3-C4	19.80	120.50	110.60
22	BA	2199	A	N1-C2-N3	-19.80	119.40	129.30
22	BA	447	A	N1-C2-N3	-19.80	119.40	129.30
22	BA	572	A	C2-N3-C4	19.80	120.50	110.60
22	BA	1244	A	C2-N3-C4	19.80	120.50	110.60
22	BA	1504	A	N1-C2-N3	-19.80	119.40	129.30
1	AA	1503	A	N1-C2-N3	-19.79	119.40	129.30
1	AA	327	A	C2-N3-C4	19.79	120.50	110.60
22	BA	1365	A	N1-C2-N3	-19.79	119.40	129.30
22	BA	2764	A	N1-C2-N3	-19.79	119.41	129.30
1	AA	321	A	C2-N3-C4	19.79	120.50	110.60
22	BA	2835	A	N1-C2-N3	-19.79	119.41	129.30
22	BA	2856	A	N1-C6-N6	-19.79	106.73	118.60
1	AA	622	A	C2-N3-C4	19.79	120.49	110.60
22	BA	1755	A	N1-C6-N6	-19.79	106.73	118.60
1	AA	374	A	N1-C2-N3	-19.78	119.41	129.30
22	BA	310	A	N1-C6-N6	-19.78	106.73	118.60
22	BA	402	A	C2-N3-C4	19.78	120.49	110.60
1	AA	1410	A	C2-N3-C4	19.78	120.49	110.60
22	BA	191	A	N1-C2-N3	-19.78	119.41	129.30
22	BA	528	A	C2-N3-C4	19.78	120.49	110.60
22	BA	1095	A	N1-C6-N6	-19.78	106.73	118.60
55	B8	41	A	C2-N3-C4	19.78	120.49	110.60
1	AA	716	A	N1-C2-N3	-19.78	119.41	129.30
22	BA	1802	A	N1-C2-N3	-19.78	119.41	129.30
22	BA	1393	A	C2-N3-C4	19.77	120.49	110.60
1	AA	131	A	C2-N3-C4	19.77	120.49	110.60
1	AA	465	A	N1-C2-N3	-19.77	119.41	129.30
22	BA	866	A	N1-C6-N6	-19.77	106.74	118.60
1	AA	630	A	C2-N3-C4	19.77	120.48	110.60
22	BA	2809	A	C2-N3-C4	19.77	120.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1204	A	N1-C2-N3	-19.77	119.42	129.30
1	AA	648	A	N1-C6-N6	-19.76	106.74	118.60
1	AA	994	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	471	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	590	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	794	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	1821	A	N1-C2-N3	-19.76	119.42	129.30
1	AA	26	A	C2-N3-C4	19.76	120.48	110.60
1	AA	364	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1040	A	C2-N3-C4	19.76	120.48	110.60
22	BA	909	A	N1-C2-N3	-19.75	119.42	129.30
22	BA	1237	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	265	A	N1-C2-N3	-19.75	119.42	129.30
22	BA	1635	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	1088	A	C2-N3-C4	19.75	120.47	110.60
22	BA	1395	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	2378	A	N1-C2-N3	-19.75	119.42	129.30
1	AA	978	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	2711	A	C2-N3-C4	19.74	120.47	110.60
1	AA	780	A	C2-N3-C4	19.74	120.47	110.60
1	AA	913	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	103	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	1504	A	C2-N3-C4	19.73	120.47	110.60
22	BA	1525	A	C2-N3-C4	19.73	120.47	110.60
1	AA	59	A	N1-C2-N3	-19.73	119.43	129.30
1	AA	510	A	N1-C2-N3	-19.73	119.44	129.30
1	AA	1042	A	C2-N3-C4	19.73	120.47	110.60
22	BA	454	A	N1-C2-N3	-19.73	119.44	129.30
22	BA	217	A	C2-N3-C4	19.73	120.46	110.60
1	AA	1476	A	C2-N3-C4	19.73	120.46	110.60
22	BA	38	A	N1-C6-N6	-19.72	106.77	118.60
22	BA	514	A	N1-C6-N6	-19.72	106.77	118.60
22	BA	101	A	C2-N3-C4	19.72	120.46	110.60
22	BA	2882	A	N1-C2-N3	-19.72	119.44	129.30
1	AA	1413	A	C2-N3-C4	19.72	120.46	110.60
23	BB	94	A	C2-N3-C4	19.72	120.46	110.60
22	BA	294	A	N1-C2-N3	-19.71	119.44	129.30
22	BA	1054	A	C2-N3-C4	19.71	120.46	110.60
1	AA	496	A	N1-C2-N3	-19.70	119.45	129.30
1	AA	1225	A	N1-C2-N3	-19.70	119.45	129.30
1	AA	435	A	N1-C2-N3	-19.70	119.45	129.30
1	AA	630	A	N1-C2-N3	-19.70	119.45	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2241	A	C2-N3-C4	19.70	120.45	110.60
22	BA	513	A	N1-C2-N3	-19.70	119.45	129.30
22	BA	1387	A	C2-N3-C4	19.70	120.45	110.60
22	BA	322	A	C2-N3-C4	19.69	120.45	110.60
22	BA	1269	A	C2-N3-C4	19.69	120.45	110.60
22	BA	532	A	N1-C6-N6	-19.69	106.78	118.60
22	BA	460	A	C2-N3-C4	19.69	120.44	110.60
22	BA	1010	A	N1-C2-N3	-19.68	119.46	129.30
1	AA	1289	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	1572	A	C2-N3-C4	19.68	120.44	110.60
22	BA	1307	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	1269	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	1393	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	83	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	1871	A	N1-C2-N3	-19.68	119.46	129.30
23	BB	53	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	1111	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	990	A	C2-N3-C4	19.67	120.44	110.60
1	AA	1492	A	C2-N3-C4	19.67	120.44	110.60
1	AA	1500	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	1545	A	N1-C2-N3	-19.67	119.47	129.30
22	BA	1772	A	C2-N3-C4	19.67	120.44	110.60
23	BB	104	A	N1-C2-N3	-19.67	119.47	129.30
1	AA	1022	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	1677	A	C2-N3-C4	19.67	120.43	110.60
22	BA	181	A	N1-C2-N3	-19.66	119.47	129.30
22	BA	480	A	C2-N3-C4	19.66	120.43	110.60
22	BA	2765	A	N1-C2-N3	-19.66	119.47	129.30
22	BA	2600	A	C2-N3-C4	19.66	120.43	110.60
1	AA	19	A	C2-N3-C4	19.66	120.43	110.60
22	BA	1717	A	N1-C6-N6	-19.66	106.81	118.60
1	AA	325	A	N1-C6-N6	-19.66	106.81	118.60
22	BA	1347	A	C2-N3-C4	19.65	120.43	110.60
22	BA	176	A	C2-N3-C4	19.65	120.43	110.60
22	BA	1126	A	N1-C2-N3	-19.65	119.47	129.30
1	AA	1500	A	N1-C2-N3	-19.65	119.47	129.30
1	AA	715	A	N1-C2-N3	-19.65	119.47	129.30
22	BA	1877	A	N1-C2-N3	-19.64	119.48	129.30
1	AA	1248	A	N1-C2-N3	-19.64	119.48	129.30
1	AA	129	A	N1-C6-N6	-19.64	106.82	118.60
22	BA	2706	A	N1-C6-N6	-19.64	106.82	118.60
1	AA	1377	A	N1-C2-N3	-19.64	119.48	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	56	A	N1-C6-N6	-19.64	106.82	118.60
22	BA	1713	A	N1-C2-N3	-19.64	119.48	129.30
22	BA	988	A	N1-C2-N3	-19.64	119.48	129.30
22	BA	2340	A	N1-C2-N3	-19.64	119.48	129.30
22	BA	866	A	N1-C2-N3	-19.63	119.48	129.30
22	BA	2311	A	N1-C6-N6	-19.63	106.82	118.60
1	AA	344	A	C2-N3-C4	19.63	120.42	110.60
1	AA	1311	A	C2-N3-C4	19.63	120.42	110.60
22	BA	2227	A	N1-C6-N6	-19.63	106.82	118.60
22	BA	2450	A	C2-N3-C4	19.63	120.42	110.60
1	AA	356	A	N1-C2-N3	-19.63	119.49	129.30
22	BA	1928	A	N1-C6-N6	-19.63	106.82	118.60
1	AA	909	A	N1-C6-N6	-19.63	106.82	118.60
22	BA	1020	A	N1-C2-N3	-19.63	119.49	129.30
1	AA	364	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	1789	A	N1-C2-N3	-19.62	119.49	129.30
1	AA	969	A	C2-N3-C4	19.62	120.41	110.60
22	BA	2212	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	1008	A	N1-C6-N6	-19.62	106.83	118.60
1	AA	149	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1494	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	750	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1755	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	2434	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	730	A	C2-N3-C4	19.61	120.41	110.60
22	BA	2003	A	C2-N3-C4	19.61	120.41	110.60
22	BA	2516	A	N1-C2-N3	-19.61	119.49	129.30
22	BA	1301	A	N1-C2-N3	-19.61	119.49	129.30
22	BA	342	A	N1-C2-N3	-19.61	119.50	129.30
22	BA	428	A	C2-N3-C4	19.61	120.41	110.60
22	BA	1127	A	N1-C2-N3	-19.61	119.50	129.30
1	AA	994	A	C2-N3-C4	19.61	120.40	110.60
22	BA	2679	A	C2-N3-C4	19.61	120.40	110.60
22	BA	89	A	N1-C6-N6	-19.61	106.84	118.60
22	BA	693	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	945	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1819	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	345	A	N1-C6-N6	-19.60	106.84	118.60
22	BA	947	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	1439	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	347	A	N1-C6-N6	-19.60	106.84	118.60
22	BA	927	A	C2-N3-C4	19.60	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	595	A	N1-C6-N6	-19.59	106.84	118.60
22	BA	2478	A	N1-C2-N3	-19.59	119.50	129.30
1	AA	1145	A	N1-C6-N6	-19.59	106.84	118.60
1	AA	263	A	C2-N3-C4	19.59	120.39	110.60
1	AA	1275	A	N1-C2-N3	-19.59	119.51	129.30
22	BA	2453	A	C2-N3-C4	19.59	120.39	110.60
22	BA	2711	A	N1-C6-N6	-19.59	106.85	118.60
1	AA	55	A	C2-N3-C4	19.59	120.39	110.60
1	AA	160	A	C2-N3-C4	19.59	120.39	110.60
1	AA	8	A	N1-C6-N6	-19.58	106.85	118.60
1	AA	1225	A	C2-N3-C4	19.58	120.39	110.60
22	BA	2740	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	1522	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	2860	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	590	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	661	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	1632	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	2042	A	C2-N3-C4	19.58	120.39	110.60
23	BB	53	A	C2-N3-C4	19.58	120.39	110.60
1	AA	792	A	N1-C6-N6	-19.58	106.85	118.60
1	AA	1499	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	528	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	794	A	C2-N3-C4	19.58	120.39	110.60
22	BA	1089	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	2749	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	721	A	N1-C2-N3	-19.57	119.51	129.30
22	BA	2274	A	N1-C6-N6	-19.57	106.86	118.60
1	AA	547	A	N1-C2-N3	-19.57	119.52	129.30
22	BA	443	A	C2-N3-C4	19.57	120.38	110.60
22	BA	631	A	C2-N3-C4	19.57	120.38	110.60
22	BA	892	A	C2-N3-C4	19.56	120.38	110.60
22	BA	2288	A	C2-N3-C4	19.56	120.38	110.60
22	BA	160	A	C2-N3-C4	19.56	120.38	110.60
22	BA	845	A	N1-C2-N3	-19.56	119.52	129.30
22	BA	1815	A	N1-C6-N6	-19.56	106.87	118.60
1	AA	539	A	C2-N3-C4	19.55	120.38	110.60
22	BA	142	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	1889	A	C2-N3-C4	19.55	120.38	110.60
23	BB	59	A	C2-N3-C4	19.55	120.38	110.60
22	BA	1876	A	C2-N3-C4	19.55	120.38	110.60
22	BA	497	A	C2-N3-C4	19.55	120.38	110.60
1	AA	1398	A	N1-C2-N3	-19.55	119.53	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	787	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	637	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	2750	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	508	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	429	A	N1-C6-N6	-19.54	106.87	118.60
22	BA	1226	A	C2-N3-C4	19.54	120.37	110.60
22	BA	1655	A	N1-C2-N3	-19.54	119.53	129.30
1	AA	466	A	C2-N3-C4	19.54	120.37	110.60
22	BA	1096	A	C2-N3-C4	19.54	120.37	110.60
22	BA	1268	A	C2-N3-C4	19.54	120.37	110.60
22	BA	1284	A	N1-C2-N3	-19.54	119.53	129.30
22	BA	2750	A	N1-C6-N6	-19.54	106.88	118.60
22	BA	603	A	N1-C6-N6	-19.54	106.88	118.60
22	BA	2088	A	N1-C2-N3	-19.54	119.53	129.30
22	BA	960	A	N1-C2-N3	-19.53	119.53	129.30
22	BA	981	A	N1-C2-N3	-19.53	119.53	129.30
22	BA	1204	A	C2-N3-C4	19.53	120.37	110.60
22	BA	2776	A	N1-C2-N3	-19.53	119.53	129.30
22	BA	1490	A	N1-C2-N3	-19.53	119.53	129.30
22	BA	2675	A	N1-C6-N6	-19.53	106.88	118.60
22	BA	1008	A	C2-N3-C4	19.53	120.36	110.60
1	AA	182	A	N1-C2-N3	-19.53	119.54	129.30
22	BA	599	A	N1-C6-N6	-19.53	106.88	118.60
1	AA	364	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	532	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	1040	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	2317	A	C2-N3-C4	19.52	120.36	110.60
1	AA	60	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	63	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	661	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	1431	A	N1-C2-N3	-19.52	119.54	129.30
1	AA	356	A	C2-N3-C4	19.52	120.36	110.60
1	AA	1362	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	1413	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	2114	A	C2-N3-C4	19.52	120.36	110.60
22	BA	2169	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	363	A	N1-C2-N3	-19.51	119.55	129.30
22	BA	1347	A	N1-C2-N3	-19.51	119.55	129.30
22	BA	644	A	C2-N3-C4	19.51	120.35	110.60
23	BB	104	A	C2-N3-C4	19.51	120.35	110.60
1	AA	152	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	2328	A	N1-C2-N3	-19.50	119.55	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	263	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	190	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	454	A	C2-N3-C4	19.50	120.35	110.60
22	BA	1032	A	C2-N3-C4	19.50	120.35	110.60
22	BA	1998	A	N1-C2-N3	-19.50	119.55	129.30
1	AA	959	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	2094	A	C2-N3-C4	19.50	120.35	110.60
1	AA	1396	A	C2-N3-C4	19.50	120.35	110.60
22	BA	1328	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	2873	A	C2-N3-C4	19.50	120.35	110.60
1	AA	414	A	N1-C2-N3	-19.49	119.55	129.30
1	AA	802	A	C2-N3-C4	19.49	120.35	110.60
23	BB	78	A	N1-C6-N6	-19.49	106.90	118.60
1	AA	1288	A	N1-C6-N6	-19.49	106.90	118.60
22	BA	94	A	N1-C2-N3	-19.49	119.55	129.30
22	BA	402	A	N1-C6-N6	-19.49	106.91	118.60
22	BA	262	A	N1-C2-N3	-19.49	119.56	129.30
22	BA	1655	A	N1-C6-N6	-19.49	106.91	118.60
22	BA	2564	A	N1-C2-N3	-19.49	119.56	129.30
1	AA	3	A	C2-N3-C4	19.48	120.34	110.60
1	AA	535	A	N1-C2-N3	-19.48	119.56	129.30
22	BA	118	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	783	A	N1-C2-N3	-19.48	119.56	129.30
22	BA	1085	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	1383	A	C2-N3-C4	19.48	120.34	110.60
22	BA	547	A	C2-N3-C4	19.48	120.34	110.60
1	AA	695	A	C2-N3-C4	19.48	120.34	110.60
22	BA	2721	A	N1-C2-N3	-19.48	119.56	129.30
1	AA	1480	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	556	A	C2-N3-C4	19.48	120.34	110.60
22	BA	751	A	N1-C2-N3	-19.48	119.56	129.30
22	BA	1103	A	N1-C2-N3	-19.48	119.56	129.30
22	BA	2358	A	N1-C6-N6	-19.48	106.92	118.60
22	BA	322	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	753	A	C2-N3-C4	19.47	120.34	110.60
1	AA	181	A	C2-N3-C4	19.47	120.34	110.60
1	AA	759	A	C2-N3-C4	19.47	120.34	110.60
22	BA	1598	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	1632	A	C2-N3-C4	19.47	120.34	110.60
22	BA	449	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	529	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	2298	A	N1-C2-N3	-19.47	119.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	718	A	N1-C2-N3	-19.47	119.57	129.30
22	BA	1634	A	N1-C2-N3	-19.47	119.57	129.30
1	AA	918	A	N1-C2-N3	-19.47	119.57	129.30
1	AA	1000	A	N1-C2-N3	-19.47	119.57	129.30
22	BA	1829	A	N1-C6-N6	-19.46	106.92	118.60
1	AA	1363	A	C2-N3-C4	19.46	120.33	110.60
22	BA	226	A	C2-N3-C4	19.46	120.33	110.60
22	BA	2639	A	N1-C6-N6	-19.46	106.92	118.60
22	BA	182	A	C2-N3-C4	19.46	120.33	110.60
22	BA	2439	A	N1-C6-N6	-19.46	106.92	118.60
1	AA	195	A	N1-C6-N6	-19.46	106.92	118.60
22	BA	83	A	C2-N3-C4	19.46	120.33	110.60
22	BA	1641	A	C2-N3-C4	19.46	120.33	110.60
22	BA	1286	A	C2-N3-C4	19.46	120.33	110.60
22	BA	2439	A	N1-C2-N3	-19.45	119.57	129.30
1	AA	864	A	N1-C2-N3	-19.45	119.57	129.30
1	AA	1179	A	C2-N3-C4	19.45	120.33	110.60
22	BA	73	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	2170	A	N1-C2-N3	-19.45	119.57	129.30
1	AA	781	A	N1-C2-N3	-19.45	119.57	129.30
22	BA	973	A	N1-C6-N6	-19.45	106.93	118.60
1	AA	389	A	C2-N3-C4	19.45	120.33	110.60
1	AA	496	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	142	A	C2-N3-C4	19.45	120.33	110.60
22	BA	439	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	592	A	N1-C2-N3	-19.45	119.58	129.30
1	AA	782	A	N1-C2-N3	-19.45	119.58	129.30
22	BA	504	A	N1-C2-N3	-19.45	119.58	129.30
22	BA	1453	A	N1-C2-N3	-19.45	119.58	129.30
1	AA	935	A	C2-N3-C4	19.44	120.32	110.60
22	BA	2376	A	C2-N3-C4	19.44	120.32	110.60
1	AA	179	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	2090	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	1098	A	N1-C6-N6	-19.43	106.94	118.60
1	AA	600	A	C2-N3-C4	19.43	120.32	110.60
22	BA	1403	A	C2-N3-C4	19.43	120.32	110.60
22	BA	668	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	845	A	N1-C6-N6	-19.43	106.94	118.60
22	BA	1735	A	C2-N3-C4	19.43	120.31	110.60
22	BA	2879	A	N1-C2-N3	-19.43	119.58	129.30
1	AA	441	A	N1-C2-N3	-19.43	119.59	129.30
22	BA	2451	A	C2-N3-C4	19.42	120.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1669	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	1717	A	N1-C2-N3	-19.42	119.59	129.30
22	BA	2541	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	2062	A	C2-N3-C4	19.42	120.31	110.60
1	AA	263	A	N1-C6-N6	-19.42	106.95	118.60
1	AA	1102	A	C2-N3-C4	19.42	120.31	110.60
22	BA	1786	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	2435	A	C2-N3-C4	19.42	120.31	110.60
1	AA	192	A	C2-N3-C4	19.42	120.31	110.60
22	BA	1749	A	C2-N3-C4	19.42	120.31	110.60
22	BA	346	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	2119	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	2432	A	N1-C2-N3	-19.41	119.59	129.30
1	AA	8	A	C2-N3-C4	19.41	120.31	110.60
22	BA	602	A	C2-N3-C4	19.41	120.31	110.60
22	BA	1552	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	1635	A	C2-N3-C4	19.41	120.31	110.60
1	AA	1410	A	N1-C2-N3	-19.41	119.60	129.30
22	BA	1477	A	N1-C2-N3	-19.41	119.60	129.30
22	BA	2448	A	C2-N3-C4	19.41	120.30	110.60
22	BA	2516	A	N1-C6-N6	-19.41	106.96	118.60
22	BA	789	A	C2-N3-C4	19.40	120.30	110.60
22	BA	1046	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	2052	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	2461	A	C2-N3-C4	19.40	120.30	110.60
1	AA	44	A	N1-C6-N6	-19.40	106.96	118.60
22	BA	311	A	N1-C6-N6	-19.40	106.96	118.60
22	BA	1525	A	N1-C2-N3	-19.40	119.60	129.30
1	AA	496	A	C2-N3-C4	19.39	120.30	110.60
22	BA	783	A	N1-C6-N6	-19.39	106.96	118.60
1	AA	1236	A	C2-N3-C4	19.39	120.30	110.60
22	BA	181	A	N1-C6-N6	-19.39	106.96	118.60
22	BA	2590	A	C2-N3-C4	19.39	120.30	110.60
1	AA	865	A	C2-N3-C4	19.39	120.30	110.60
22	BA	1598	A	C2-N3-C4	19.39	120.30	110.60
1	AA	681	A	N1-C2-N3	-19.39	119.61	129.30
22	BA	1367	A	N1-C2-N3	-19.39	119.61	129.30
1	AA	344	A	N1-C2-N3	-19.39	119.61	129.30
1	AA	459	A	C2-N3-C4	19.39	120.29	110.60
22	BA	943	A	C2-N3-C4	19.39	120.29	110.60
22	BA	1129	A	N1-C6-N6	-19.39	106.97	118.60
22	BA	2327	A	N1-C2-N3	-19.39	119.61	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	608	A	N1-C2-N3	-19.38	119.61	129.30
1	AA	673	A	C2-N3-C4	19.38	120.29	110.60
1	AA	1196	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	176	A	N1-C2-N3	-19.38	119.61	129.30
1	AA	60	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	1050	A	C2-N3-C4	19.38	120.29	110.60
22	BA	219	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	330	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	1134	A	N1-C2-N3	-19.37	119.61	129.30
1	AA	338	A	C2-N3-C4	19.37	120.29	110.60
1	AA	7	A	C2-N3-C4	19.37	120.28	110.60
22	BA	213	A	N1-C6-N6	-19.37	106.98	118.60
1	AA	1357	A	N1-C2-N3	-19.37	119.62	129.30
22	BA	1586	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	471	A	C2-N3-C4	19.36	120.28	110.60
1	AA	7	A	N1-C2-N3	-19.36	119.62	129.30
1	AA	7	A	N1-C6-N6	-19.36	106.98	118.60
1	AA	309	A	N1-C6-N6	-19.36	106.98	118.60
22	BA	909	A	C2-N3-C4	19.36	120.28	110.60
1	AA	1042	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	753	A	N1-C6-N6	-19.36	106.98	118.60
1	AA	815	A	N1-C2-N3	-19.36	119.62	129.30
1	AA	1447	A	N1-C6-N6	-19.36	106.98	118.60
1	AA	65	A	N1-C2-N3	-19.36	119.62	129.30
1	AA	583	A	N1-C6-N6	-19.36	106.99	118.60
22	BA	1322	A	N1-C6-N6	-19.36	106.99	118.60
22	BA	2814	A	N1-C6-N6	-19.36	106.99	118.60
1	AA	321	A	N1-C2-N3	-19.36	119.62	129.30
1	AA	1329	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	1247	A	C2-N3-C4	19.35	120.28	110.60
22	BA	430	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	1803	A	C2-N3-C4	19.35	120.28	110.60
1	AA	825	A	C2-N3-C4	19.35	120.28	110.60
22	BA	1085	A	C2-N3-C4	19.35	120.27	110.60
1	AA	71	A	C2-N3-C4	19.35	120.27	110.60
22	BA	131	A	N1-C2-N3	-19.35	119.63	129.30
22	BA	1549	A	C2-N3-C4	19.35	120.27	110.60
22	BA	14	A	C2-N3-C4	19.34	120.27	110.60
22	BA	449	A	N1-C6-N6	-19.34	106.99	118.60
22	BA	322	A	N1-C6-N6	-19.34	107.00	118.60
1	AA	908	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	118	A	N1-C2-N3	-19.34	119.63	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1395	A	C2-N3-C4	19.34	120.27	110.60
22	BA	1938	A	C2-N3-C4	19.34	120.27	110.60
22	BA	2037	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	1502	A	N1-C2-N3	-19.34	119.63	129.30
1	AA	151	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	344	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	1433	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	1373	A	C2-N3-C4	19.33	120.27	110.60
22	BA	2314	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2088	A	C2-N3-C4	19.33	120.26	110.60
22	BA	2418	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2761	A	N1-C2-N3	-19.33	119.64	129.30
1	AA	16	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	1705	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	1340	A	N1-C6-N6	-19.32	107.00	118.60
22	BA	111	A	C2-N3-C4	19.32	120.26	110.60
1	AA	816	A	C2-N3-C4	19.32	120.26	110.60
1	AA	1319	A	N1-C2-N3	-19.32	119.64	129.30
1	AA	1333	A	C2-N3-C4	19.32	120.26	110.60
22	BA	1780	A	C2-N3-C4	19.32	120.26	110.60
22	BA	2135	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	2247	A	C2-N3-C4	19.32	120.26	110.60
1	AA	819	A	N1-C2-N3	-19.32	119.64	129.30
1	AA	1092	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	262	A	C2-N3-C4	19.32	120.26	110.60
22	BA	1098	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	222	A	N1-C6-N6	-19.32	107.01	118.60
1	AA	958	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	1901	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	219	A	C2-N3-C4	19.31	120.26	110.60
22	BA	928	A	C2-N3-C4	19.31	120.26	110.60
1	AA	1239	A	N1-C2-N3	-19.31	119.64	129.30
22	BA	715	A	N1-C2-N3	-19.31	119.64	129.30
22	BA	1069	A	N1-C6-N6	-19.31	107.01	118.60
1	AA	298	A	N1-C2-N3	-19.31	119.64	129.30
22	BA	49	A	C2-N3-C4	19.31	120.25	110.60
22	BA	2328	A	C2-N3-C4	19.31	120.25	110.60
22	BA	2813	A	C2-N3-C4	19.31	120.25	110.60
23	BB	109	A	N1-C2-N3	-19.31	119.65	129.30
22	BA	655	A	N1-C2-N3	-19.31	119.65	129.30
23	BB	94	A	N1-C6-N6	-19.31	107.02	118.60
1	AA	363	A	N1-C6-N6	-19.31	107.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	397	A	N1-C2-N3	-19.31	119.65	129.30
22	BA	522	A	N1-C2-N3	-19.31	119.65	129.30
22	BA	632	A	N1-C2-N3	-19.31	119.65	129.30
22	BA	988	A	N1-C6-N6	-19.31	107.02	118.60
22	BA	2274	A	N1-C2-N3	-19.31	119.65	129.30
22	BA	900	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	2826	A	C2-N3-C4	19.30	120.25	110.60
22	BA	1654	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	1866	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	1032	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	1103	A	C2-N3-C4	19.30	120.25	110.60
22	BA	1490	A	C2-N3-C4	19.29	120.25	110.60
22	BA	472	A	N1-C2-N3	-19.29	119.65	129.30
22	BA	676	A	N1-C6-N6	-19.29	107.02	118.60
22	BA	1260	A	C2-N3-C4	19.29	120.25	110.60
1	AA	228	A	N1-C2-N3	-19.29	119.66	129.30
1	AA	935	A	N1-C6-N6	-19.29	107.03	118.60
1	AA	1117	A	N1-C2-N3	-19.29	119.66	129.30
1	AA	1204	A	N1-C6-N6	-19.29	107.03	118.60
1	AA	1410	A	N1-C6-N6	-19.29	107.03	118.60
1	AA	1236	A	N1-C2-N3	-19.29	119.66	129.30
1	AA	1319	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	216	A	C2-N3-C4	19.28	120.24	110.60
22	BA	1593	A	C2-N3-C4	19.28	120.24	110.60
1	AA	28	A	C2-N3-C4	19.28	120.24	110.60
1	AA	892	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	1096	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	1384	A	C2-N3-C4	19.28	120.24	110.60
22	BA	2014	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	2530	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	2706	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	156	A	C2-N3-C4	19.28	120.24	110.60
22	BA	2082	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	2117	A	C2-N3-C4	19.28	120.24	110.60
22	BA	478	A	C2-N3-C4	19.27	120.24	110.60
23	BB	108	A	C2-N3-C4	19.27	120.24	110.60
1	AA	520	A	N1-C2-N3	-19.27	119.66	129.30
22	BA	614	A	N1-C2-N3	-19.27	119.66	129.30
22	BA	1090	A	C2-N3-C4	19.27	120.24	110.60
22	BA	2778	A	C2-N3-C4	19.27	120.24	110.60
22	BA	2727	A	C2-N3-C4	19.27	120.23	110.60
22	BA	1387	A	N1-C2-N3	-19.27	119.67	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	336	A	N1-C6-N6	-19.27	107.04	118.60
1	AA	865	A	N1-C6-N6	-19.27	107.04	118.60
1	AA	958	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	89	A	C2-N3-C4	19.27	120.23	110.60
22	BA	118	A	C2-N3-C4	19.27	120.23	110.60
22	BA	1745	A	N1-C2-N3	-19.27	119.67	129.30
22	BA	2425	A	C2-N3-C4	19.27	120.23	110.60
22	BA	1304	A	N1-C6-N6	-19.26	107.04	118.60
22	BA	2873	A	N1-C6-N6	-19.26	107.04	118.60
1	AA	77	A	C2-N3-C4	19.26	120.23	110.60
22	BA	911	A	C2-N3-C4	19.26	120.23	110.60
22	BA	2516	A	C2-N3-C4	19.26	120.23	110.60
22	BA	300	A	C2-N3-C4	19.26	120.23	110.60
22	BA	1505	A	N1-C6-N6	-19.26	107.05	118.60
22	BA	1928	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	1535	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	2154	A	N1-C6-N6	-19.26	107.05	118.60
1	AA	845	A	C2-N3-C4	19.25	120.23	110.60
22	BA	1254	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	2682	A	C2-N3-C4	19.25	120.23	110.60
1	AA	816	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	241	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1900	A	C2-N3-C4	19.25	120.23	110.60
1	AA	892	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	53	A	C2-N3-C4	19.25	120.23	110.60
22	BA	1890	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	2058	A	C2-N3-C4	19.25	120.23	110.60
1	AA	1005	A	C2-N3-C4	19.25	120.22	110.60
22	BA	1427	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	2211	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	1583	A	C2-N3-C4	19.25	120.22	110.60
22	BA	1669	A	N1-C2-N3	-19.25	119.67	129.30
1	AA	431	A	N1-C2-N3	-19.25	119.68	129.30
1	AA	889	A	N1-C2-N3	-19.25	119.68	129.30
22	BA	190	A	C2-N3-C4	19.25	120.22	110.60
1	AA	1394	A	N1-C2-N3	-19.25	119.68	129.30
22	BA	1165	A	C2-N3-C4	19.25	120.22	110.60
22	BA	1544	A	N1-C6-N6	-19.25	107.05	118.60
1	AA	223	A	N1-C6-N6	-19.24	107.06	118.60
22	BA	2314	A	C2-N3-C4	19.24	120.22	110.60
1	AA	794	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	345	A	N1-C2-N3	-19.24	119.68	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1492	A	N1-C6-N6	-19.24	107.06	118.60
22	BA	42	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	299	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	627	A	C2-N3-C4	19.24	120.22	110.60
22	BA	1272	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	1744	A	N1-C6-N6	-19.24	107.06	118.60
22	BA	2054	A	C2-N3-C4	19.24	120.22	110.60
1	AA	602	A	C2-N3-C4	19.23	120.22	110.60
1	AA	864	A	C2-N3-C4	19.23	120.22	110.60
1	AA	1081	A	N1-C2-N3	-19.23	119.68	129.30
1	AA	676	A	N1-C2-N3	-19.23	119.68	129.30
22	BA	800	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	1746	A	N1-C6-N6	-19.23	107.06	118.60
1	AA	499	A	C2-N3-C4	19.23	120.21	110.60
22	BA	422	A	C2-N3-C4	19.23	120.21	110.60
22	BA	892	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	2080	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	332	A	C2-N3-C4	19.22	120.21	110.60
1	AA	872	A	C2-N3-C4	19.21	120.21	110.60
22	BA	1597	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	1701	A	C2-N3-C4	19.21	120.21	110.60
22	BA	1785	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	1287	A	C2-N3-C4	19.21	120.21	110.60
1	AA	1012	A	C2-N3-C4	19.21	120.21	110.60
22	BA	616	A	C2-N3-C4	19.21	120.21	110.60
22	BA	2388	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	1353	A	N1-C6-N6	-19.21	107.08	118.60
1	AA	149	A	C2-N3-C4	19.21	120.20	110.60
1	AA	139	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	665	A	N1-C6-N6	-19.20	107.08	118.60
1	AA	130	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	336	A	C2-N3-C4	19.20	120.20	110.60
1	AA	602	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	696	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	250	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	1597	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	2015	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	282	A	N1-C6-N6	-19.20	107.08	118.60
1	AA	915	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	2336	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	2700	A	N1-C6-N6	-19.19	107.08	118.60
1	AA	448	A	N1-C2-N3	-19.19	119.70	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1456	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	13	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	1783	A	N1-C6-N6	-19.19	107.08	118.60
22	BA	1503	A	C2-N3-C4	19.19	120.19	110.60
22	BA	2851	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	1522	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	1590	A	C2-N3-C4	19.19	120.19	110.60
1	AA	119	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	1912	A	N1-C6-N6	-19.19	107.09	118.60
1	AA	493	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	626	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	320	A	N1-C6-N6	-19.18	107.09	118.60
1	AA	3	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	975	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	2	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	2738	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	600	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	1150	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	583	A	N1-C2-N3	-19.17	119.71	129.30
22	BA	1970	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	2147	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	2662	A	C2-N3-C4	19.17	120.19	110.60
1	AA	595	A	C2-N3-C4	19.17	120.18	110.60
1	AA	675	A	N1-C6-N6	-19.16	107.10	118.60
22	BA	1650	A	C2-N3-C4	19.16	120.18	110.60
1	AA	687	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	2632	A	C2-N3-C4	19.16	120.18	110.60
22	BA	1591	A	N1-C2-N3	-19.16	119.72	129.30
1	AA	78	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	2706	A	C2-N3-C4	19.16	120.18	110.60
1	AA	327	A	N1-C6-N6	-19.16	107.11	118.60
1	AA	777	A	N1-C2-N3	-19.15	119.72	129.30
22	BA	218	A	N1-C2-N3	-19.15	119.72	129.30
1	AA	315	A	C2-N3-C4	19.15	120.17	110.60
54	B7	9	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	627	A	N1-C2-N3	-19.15	119.73	129.30
23	BB	50	A	N1-C2-N3	-19.15	119.73	129.30
22	BA	1890	A	N1-C6-N6	-19.14	107.11	118.60
22	BA	1913	A	N1-C2-N3	-19.14	119.73	129.30
1	AA	607	A	C2-N3-C4	19.14	120.17	110.60
22	BA	300	A	N1-C6-N6	-19.14	107.12	118.60
22	BA	1126	A	C2-N3-C4	19.14	120.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1276	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	1749	A	N1-C6-N6	-19.14	107.11	118.60
22	BA	480	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	718	A	N1-C6-N6	-19.14	107.12	118.60
22	BA	1420	A	C2-N3-C4	19.14	120.17	110.60
1	AA	274	A	N1-C6-N6	-19.14	107.12	118.60
1	AA	313	A	N1-C6-N6	-19.14	107.12	118.60
22	BA	2560	A	C2-N3-C4	19.14	120.17	110.60
1	AA	189	A	C2-N3-C4	19.13	120.17	110.60
1	AA	1179	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1213	A	C2-N3-C4	19.13	120.17	110.60
1	AA	560	A	N1-C6-N6	-19.13	107.12	118.60
1	AA	1534	A	N1-C2-N3	-19.13	119.73	129.30
1	AA	313	A	C2-N3-C4	19.13	120.17	110.60
22	BA	727	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1505	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	161	A	N1-C2-N3	-19.13	119.74	129.30
1	AA	1246	A	N1-C2-N3	-19.13	119.74	129.30
1	AA	315	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	414	A	C2-N3-C4	19.12	120.16	110.60
22	BA	2418	A	C2-N3-C4	19.12	120.16	110.60
1	AA	914	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	964	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	1437	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1088	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	2813	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1378	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1096	A	N1-C2-N3	-19.11	119.74	129.30
22	BA	563	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	979	A	N1-C2-N3	-19.11	119.74	129.30
22	BA	1009	A	C2-N3-C4	19.11	120.16	110.60
1	AA	509	A	C2-N3-C4	19.11	120.16	110.60
1	AA	787	A	C2-N3-C4	19.11	120.16	110.60
1	AA	1145	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	866	A	C2-N3-C4	19.11	120.15	110.60
1	AA	303	A	C2-N3-C4	19.11	120.15	110.60
22	BA	877	A	N1-C6-N6	-19.11	107.14	118.60
1	AA	262	A	N1-C2-N3	-19.11	119.75	129.30
1	AA	1318	A	N1-C2-N3	-19.11	119.75	129.30
1	AA	694	A	C2-N3-C4	19.10	120.15	110.60
22	BA	1155	A	N1-C2-N3	-19.10	119.75	129.30
22	BA	2212	A	C2-N3-C4	19.10	120.15	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	231	A	N1-C2-N3	-19.10	119.75	129.30
22	BA	1632	A	N1-C6-N6	-19.10	107.14	118.60
22	BA	2749	A	C2-N3-C4	19.10	120.15	110.60
1	AA	935	A	N1-C2-N3	-19.10	119.75	129.30
1	AA	1431	A	N1-C6-N6	-19.10	107.14	118.60
55	B8	42	A	N1-C6-N6	-19.10	107.14	118.60
22	BA	878	A	N1-C2-N3	-19.10	119.75	129.30
1	AA	1360	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	204	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	2829	A	C2-N3-C4	19.09	120.14	110.60
22	BA	1373	A	N1-C2-N3	-19.09	119.76	129.30
22	BA	2090	A	C2-N3-C4	19.09	120.14	110.60
22	BA	10	A	N1-C2-N3	-19.09	119.76	129.30
23	BB	15	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	1700	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	1981	A	N1-C2-N3	-19.08	119.76	129.30
55	B8	73	A	N1-C6-N6	-19.08	107.15	118.60
1	AA	65	A	C2-N3-C4	19.08	120.14	110.60
22	BA	347	A	C2-N3-C4	19.08	120.14	110.60
22	BA	1434	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	2541	A	N1-C2-N3	-19.08	119.76	129.30
55	B8	26	A	C2-N3-C4	19.08	120.14	110.60
1	AA	412	A	N1-C6-N6	-19.08	107.15	118.60
1	AA	1319	A	C2-N3-C4	19.08	120.14	110.60
55	B8	14	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	716	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	1155	A	C2-N3-C4	19.07	120.14	110.60
55	B8	21	A	N1-C2-N3	-19.07	119.76	129.30
1	AA	1167	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	849	A	N1-C2-N3	-19.07	119.77	129.30
1	AA	1441	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	1254	A	C2-N3-C4	19.07	120.13	110.60
23	BB	46	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	189	A	N1-C6-N6	-19.06	107.16	118.60
22	BA	478	A	N1-C2-N3	-19.06	119.77	129.30
1	AA	906	A	C2-N3-C4	19.06	120.13	110.60
1	AA	1429	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	655	A	C2-N3-C4	19.06	120.13	110.60
1	AA	1252	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	905	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	1678	A	C2-N3-C4	19.06	120.13	110.60
22	BA	2757	A	C2-N3-C4	19.06	120.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	579	A	N1-C2-N3	-19.05	119.77	129.30
22	BA	980	A	N1-C2-N3	-19.05	119.77	129.30
22	BA	586	A	N1-C2-N3	-19.05	119.77	129.30
23	BB	39	A	C2-N3-C4	19.05	120.13	110.60
1	AA	1044	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	64	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	311	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	1918	A	N1-C6-N6	-19.05	107.17	118.60
23	BB	108	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	814	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	1271	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	556	A	N1-C6-N6	-19.04	107.17	118.60
22	BA	2565	A	N1-C2-N3	-19.04	119.78	129.30
55	B8	14	A	C2-N3-C4	19.04	120.12	110.60
1	AA	1340	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	1349	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	1357	A	N1-C6-N6	-19.04	107.18	118.60
1	AA	1446	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1952	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	146	A	C2-N3-C4	19.04	120.12	110.60
22	BA	631	A	N1-C6-N6	-19.04	107.18	118.60
22	BA	294	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1749	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	262	A	C2-N3-C4	19.03	120.12	110.60
22	BA	2826	A	N1-C6-N6	-19.03	107.18	118.60
1	AA	448	A	C2-N3-C4	19.03	120.12	110.60
22	BA	1067	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	1237	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	788	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	899	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	1690	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	2266	A	C2-N3-C4	19.03	120.12	110.60
1	AA	1375	A	C2-N3-C4	19.03	120.11	110.60
22	BA	2088	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	2564	A	C2-N3-C4	19.02	120.11	110.60
22	BA	911	A	N1-C2-N3	-19.02	119.79	129.30
1	AA	1151	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1889	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	2135	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	71	A	N1-C2-N3	-19.02	119.79	129.30
1	AA	908	A	C2-N3-C4	19.01	120.11	110.60
1	AA	1180	A	C2-N3-C4	19.01	120.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2476	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	722	A	C2-N3-C4	19.01	120.11	110.60
1	AA	101	A	C2-N3-C4	19.01	120.11	110.60
1	AA	196	A	C2-N3-C4	19.01	120.11	110.60
1	AA	546	A	C2-N3-C4	19.01	120.11	110.60
1	AA	574	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	1322	A	C2-N3-C4	19.01	120.11	110.60
22	BA	1889	A	N1-C2-N3	-19.01	119.80	129.30
22	BA	2333	A	N1-C2-N3	-19.01	119.80	129.30
23	BB	39	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	547	A	N1-C6-N6	-19.01	107.20	118.60
22	BA	1175	A	N1-C2-N3	-19.01	119.80	129.30
1	AA	435	A	C2-N3-C4	19.00	120.10	110.60
1	AA	595	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2733	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	1794	A	C2-N3-C4	19.00	120.10	110.60
1	AA	1492	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	59	A	C2-N3-C4	19.00	120.10	110.60
1	AA	1188	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2117	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	51	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	1340	A	C2-N3-C4	19.00	120.10	110.60
22	BA	1700	A	N1-C2-N3	-18.99	119.80	129.30
22	BA	470	A	C2-N3-C4	18.99	120.10	110.60
1	AA	1191	A	N1-C2-N3	-18.99	119.81	129.30
22	BA	1039	A	C2-N3-C4	18.99	120.09	110.60
22	BA	1383	A	N1-C2-N3	-18.99	119.81	129.30
1	AA	1016	A	C2-N3-C4	18.99	120.09	110.60
55	B8	42	A	C2-N3-C4	18.99	120.09	110.60
1	AA	918	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2019	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	2883	A	C2-N3-C4	18.98	120.09	110.60
22	BA	507	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	1101	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	324	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	1246	A	C2-N3-C4	18.98	120.09	110.60
1	AA	205	A	C2-N3-C4	18.98	120.09	110.60
1	AA	68	G	C8-N9-C4	-18.98	98.81	106.40
1	AA	196	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	2534	A	C2-N3-C4	18.98	120.09	110.60
1	AA	274	A	C2-N3-C4	18.98	120.09	110.60
1	AA	523	A	N1-C2-N3	-18.98	119.81	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1016	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	477	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2014	A	N1-C6-N6	-18.98	107.21	118.60
1	AA	1	A	N1-C6-N6	-18.97	107.22	118.60
1	AA	412	A	N1-C2-N3	-18.97	119.81	129.30
22	BA	1509	A	N1-C2-N3	-18.97	119.81	129.30
22	BA	165	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	661	A	C2-N3-C4	18.97	120.08	110.60
22	BA	1515	A	N1-C2-N3	-18.97	119.82	129.30
22	BA	470	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	1640	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2333	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1205	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	1549	A	N1-C2-N3	-18.96	119.82	129.30
1	AA	270	A	C2-N3-C4	18.96	120.08	110.60
1	AA	451	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1098	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2566	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1387	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	1689	A	N1-C2-N3	-18.95	119.82	129.30
55	B8	21	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	83	A	N1-C6-N6	-18.95	107.23	118.60
1	AA	338	A	N1-C2-N3	-18.95	119.83	129.30
1	AA	320	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	815	A	C2-N3-C4	18.94	120.07	110.60
1	AA	161	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	609	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	729	A	C2-N3-C4	18.94	120.07	110.60
22	BA	1302	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	907	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	151	A	C2-N3-C4	18.94	120.07	110.60
1	AA	958	A	C2-N3-C4	18.94	120.07	110.60
22	BA	226	A	N1-C6-N6	-18.94	107.24	118.60
1	AA	149	A	N1-C2-N3	-18.93	119.83	129.30
1	AA	864	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	430	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	613	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	920	A	C2-N3-C4	18.93	120.07	110.60
22	BA	1301	A	C2-N3-C4	18.93	120.07	110.60
22	BA	1978	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	373	A	C2-N3-C4	18.93	120.06	110.60
22	BA	2158	A	N1-C2-N3	-18.93	119.83	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1398	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	751	A	C2-N3-C4	18.93	120.06	110.60
22	BA	1966	A	C2-N3-C4	18.93	120.06	110.60
22	BA	447	A	N1-C6-N6	-18.93	107.25	118.60
1	AA	60	A	C2-N3-C4	18.92	120.06	110.60
1	AA	171	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	172	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	1275	A	C2-N3-C4	18.92	120.06	110.60
1	AA	243	A	C2-N3-C4	18.92	120.06	110.60
1	AA	608	A	C2-N3-C4	18.92	120.06	110.60
1	AA	1146	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	219	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	1815	A	C2-N3-C4	18.92	120.06	110.60
22	BA	1938	A	N1-C2-N3	-18.92	119.84	129.30
23	BB	52	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	74	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	1717	A	C2-N3-C4	18.92	120.06	110.60
1	AA	1362	A	C2-N3-C4	18.92	120.06	110.60
1	AA	539	A	N1-C2-N3	-18.91	119.84	129.30
22	BA	718	A	C2-N3-C4	18.91	120.06	110.60
22	BA	905	A	C2-N3-C4	18.91	120.06	110.60
22	BA	1713	A	C2-N3-C4	18.91	120.06	110.60
1	AA	768	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	1586	A	N1-C2-N3	-18.91	119.84	129.30
22	BA	2800	A	C2-N3-C4	18.91	120.06	110.60
22	BA	2009	A	C2-N3-C4	18.91	120.06	110.60
22	BA	2810	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	1000	A	C2-N3-C4	18.91	120.05	110.60
1	AA	456	A	C2-N3-C4	18.90	120.05	110.60
1	AA	431	A	C2-N3-C4	18.90	120.05	110.60
1	AA	675	A	C2-N3-C4	18.90	120.05	110.60
1	AA	949	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1871	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1744	A	C2-N3-C4	18.90	120.05	110.60
1	AA	236	A	C2-N3-C4	18.90	120.05	110.60
22	BA	28	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	749	A	C2-N3-C4	18.90	120.05	110.60
22	BA	2388	A	C2-N3-C4	18.90	120.05	110.60
22	BA	2781	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1679	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1829	A	N1-C2-N3	-18.90	119.85	129.30
23	BB	15	A	N1-C6-N6	-18.90	107.26	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1014	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1036	A	N1-C6-N6	-18.89	107.26	118.60
22	BA	752	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	1698	A	N1-C6-N6	-18.89	107.26	118.60
22	BA	2335	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	735	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	1669	A	C2-N3-C4	18.89	120.05	110.60
1	AA	246	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	1127	A	C2-N3-C4	18.89	120.04	110.60
22	BA	1608	A	C2-N3-C4	18.89	120.04	110.60
22	BA	1919	A	N1-C6-N6	-18.89	107.27	118.60
1	AA	366	A	C2-N3-C4	18.89	120.04	110.60
1	AA	1022	A	C2-N3-C4	18.89	120.04	110.60
22	BA	173	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	479	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	861	A	C2-N3-C4	18.89	120.04	110.60
22	BA	2333	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	44	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	466	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	946	A	C2-N3-C4	18.88	120.04	110.60
22	BA	802	A	N1-C2-N3	-18.88	119.86	129.30
1	AA	50	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	116	A	N1-C2-N3	-18.88	119.86	129.30
1	AA	382	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	2590	A	N1-C6-N6	-18.88	107.27	118.60
55	B8	58	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1359	A	N1-C2-N3	-18.88	119.86	129.30
55	B8	6	A	N1-C2-N3	-18.87	119.86	129.30
22	BA	633	A	N1-C2-N3	-18.87	119.86	129.30
22	BA	863	A	N1-C2-N3	-18.87	119.86	129.30
22	BA	2726	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	344	A	N1-C2-N3	-18.87	119.87	129.30
1	AA	109	A	C2-N3-C4	18.86	120.03	110.60
1	AA	559	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1513	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2198	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2513	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	120	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	155	A	C2-N3-C4	18.86	120.03	110.60
22	BA	706	A	C2-N3-C4	18.86	120.03	110.60
1	AA	109	A	N1-C6-N6	-18.86	107.28	118.60
1	AA	648	A	C2-N3-C4	18.86	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1269	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1070	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	739	A	C2-N3-C4	18.86	120.03	110.60
1	AA	456	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	294	A	N1-C6-N6	-18.86	107.29	118.60
22	BA	973	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	532	A	N1-C6-N6	-18.86	107.29	118.60
22	BA	793	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	1036	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	1858	A	N1-C2-N3	-18.85	119.87	129.30
1	AA	174	A	C2-N3-C4	18.85	120.03	110.60
1	AA	1428	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	1784	A	C2-N3-C4	18.85	120.03	110.60
22	BA	265	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	1133	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	2060	A	C2-N3-C4	18.85	120.03	110.60
1	AA	746	A	C2-N3-C4	18.85	120.03	110.60
22	BA	2191	A	C2-N3-C4	18.85	120.02	110.60
1	AA	648	A	N1-C2-N3	-18.85	119.88	129.30
1	AA	747	A	C2-N3-C4	18.85	120.02	110.60
1	AA	1080	A	N1-C2-N3	-18.85	119.88	129.30
1	AA	1	A	C2-N3-C4	18.85	120.02	110.60
22	BA	1890	A	C2-N3-C4	18.85	120.02	110.60
22	BA	2721	A	C2-N3-C4	18.85	120.02	110.60
1	AA	143	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1157	A	C2-N3-C4	18.84	120.02	110.60
22	BA	849	A	C2-N3-C4	18.84	120.02	110.60
22	BA	910	A	C2-N3-C4	18.84	120.02	110.60
22	BA	2660	A	N1-C6-N6	-18.84	107.29	118.60
22	BA	2478	A	N1-C6-N6	-18.84	107.29	118.60
1	AA	397	A	N1-C6-N6	-18.84	107.30	118.60
1	AA	768	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1219	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1229	A	N1-C6-N6	-18.84	107.30	118.60
22	BA	155	A	C2-N3-C4	18.84	120.02	110.60
1	AA	2	A	C2-N3-C4	18.84	120.02	110.60
1	AA	635	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	374	A	N1-C6-N6	-18.84	107.30	118.60
1	AA	451	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	529	A	C2-N3-C4	18.84	120.02	110.60
22	BA	1050	A	N1-C6-N6	-18.84	107.30	118.60
22	BA	1614	A	N1-C2-N3	-18.84	119.88	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1780	A	N1-C2-N3	-18.84	119.88	129.30
23	BB	58	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1465	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	983	A	C2-N3-C4	18.83	120.02	110.60
1	AA	695	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	702	A	C2-N3-C4	18.83	120.02	110.60
22	BA	1664	A	C2-N3-C4	18.83	120.02	110.60
22	BA	352	A	N1-C2-N3	-18.83	119.89	129.30
1	AA	1250	A	N1-C2-N3	-18.83	119.89	129.30
1	AA	1339	A	C2-N3-C4	18.83	120.01	110.60
22	BA	2886	A	N1-C2-N3	-18.83	119.89	129.30
23	BB	50	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	2227	A	C2-N3-C4	18.83	120.01	110.60
1	AA	182	A	C2-N3-C4	18.82	120.01	110.60
22	BA	1284	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	2851	A	C2-N3-C4	18.82	120.01	110.60
22	BA	272	A	C2-N3-C4	18.82	120.01	110.60
22	BA	492	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	975	A	C2-N3-C4	18.82	120.01	110.60
22	BA	73	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	265	A	C2-N3-C4	18.82	120.01	110.60
22	BA	764	A	C2-N3-C4	18.82	120.01	110.60
22	BA	820	A	C2-N3-C4	18.82	120.01	110.60
1	AA	946	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	821	A	C2-N3-C4	18.81	120.01	110.60
1	AA	325	A	C2-N3-C4	18.81	120.01	110.60
1	AA	1333	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	227	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	973	A	C2-N3-C4	18.81	120.01	110.60
22	BA	2534	A	N1-C2-N3	-18.81	119.89	129.30
1	AA	250	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	2814	A	C2-N3-C4	18.81	120.00	110.60
22	BA	2872	A	C2-N3-C4	18.81	120.00	110.60
1	AA	28	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	676	A	C2-N3-C4	18.81	120.00	110.60
22	BA	203	A	N1-C6-N6	-18.81	107.32	118.60
22	BA	936	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	468	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	142	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1081	A	C2-N3-C4	18.80	120.00	110.60
22	BA	905	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	2778	A	N1-C2-N3	-18.80	119.90	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	974	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1465	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1545	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	366	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1480	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	2020	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1044	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1028	A	C2-N3-C4	18.79	120.00	110.60
22	BA	1569	A	C2-N3-C4	18.79	120.00	110.60
1	AA	336	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1437	A	N1-C6-N6	-18.79	107.33	118.60
22	BA	1285	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1261	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1493	A	C2-N3-C4	18.79	119.99	110.60
22	BA	668	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	1151	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	563	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	1969	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1155	A	C2-N3-C4	18.79	119.99	110.60
22	BA	2205	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1252	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1987	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2513	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1248	A	N1-C6-N6	-18.78	107.33	118.60
22	BA	1609	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2565	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2287	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2205	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	909	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	1548	A	C2-N3-C4	18.78	119.99	110.60
55	B8	38	A	N1-C6-N6	-18.77	107.33	118.60
55	B8	41	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	892	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1014	A	N1-C2-N3	-18.77	119.91	129.30
22	BA	928	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	429	A	N1-C2-N3	-18.77	119.92	129.30
22	BA	1630	A	N1-C2-N3	-18.77	119.92	129.30
22	BA	666	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	1241	A	C2-N3-C4	18.77	119.98	110.60
22	BA	2534	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	478	A	C2-N3-C4	18.77	119.98	110.60
22	BA	454	A	N1-C6-N6	-18.77	107.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1901	A	C2-N3-C4	18.77	119.98	110.60
22	BA	1616	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	2314	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	315	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	172	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	2071	A	C2-N3-C4	18.76	119.98	110.60
1	AA	189	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	412	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1280	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	1346	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	1630	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1194	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2171	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	253	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	2757	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1441	A	C2-N3-C4	18.76	119.98	110.60
22	BA	44	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1434	A	N1-C2-N3	-18.75	119.92	129.30
22	BA	1039	A	N1-C6-N6	-18.75	107.35	118.60
55	B8	66	A	C2-N3-C4	18.75	119.98	110.60
1	AA	768	A	C2-N3-C4	18.75	119.98	110.60
22	BA	2163	A	N1-C2-N3	-18.75	119.92	129.30
22	BA	221	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	1913	A	C2-N3-C4	18.75	119.97	110.60
22	BA	1413	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1005	A	N1-C6-N6	-18.74	107.35	118.60
22	BA	94	A	N1-C6-N6	-18.74	107.35	118.60
22	BA	1877	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2154	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2829	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	906	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1912	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1505	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2031	A	N1-C6-N6	-18.74	107.36	118.60
55	B8	51	A	C2-N3-C4	18.74	119.97	110.60
1	AA	16	A	C2-N3-C4	18.74	119.97	110.60
22	BA	788	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1143	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1596	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	919	A	N1-C2-N3	-18.73	119.93	129.30
22	BA	582	A	C2-N3-C4	18.73	119.97	110.60
22	BA	632	A	C2-N3-C4	18.73	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1819	A	N1-C6-N6	-18.73	107.36	118.60
1	AA	1216	A	N1-C2-N3	-18.73	119.94	129.30
22	BA	761	A	C2-N3-C4	18.73	119.97	110.60
22	BA	103	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	2814	A	N1-C2-N3	-18.73	119.94	129.30
22	BA	2097	A	C2-N3-C4	18.73	119.96	110.60
1	AA	600	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	1197	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	13	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	382	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1265	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1679	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1791	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	819	A	C2-N3-C4	18.72	119.96	110.60
22	BA	231	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1134	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1147	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1205	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1214	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1652	A	C2-N3-C4	18.72	119.96	110.60
22	BA	2311	A	C2-N3-C4	18.72	119.96	110.60
1	AA	574	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	996	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	1773	A	C2-N3-C4	18.72	119.96	110.60
1	AA	152	A	C2-N3-C4	18.71	119.96	110.60
22	BA	1603	A	C2-N3-C4	18.71	119.96	110.60
1	AA	696	A	C2-N3-C4	18.71	119.96	110.60
1	AA	784	A	C2-N3-C4	18.71	119.96	110.60
1	AA	1377	A	C2-N3-C4	18.71	119.96	110.60
22	BA	1853	A	C2-N3-C4	18.71	119.96	110.60
1	AA	655	A	C2-N3-C4	18.71	119.96	110.60
22	BA	608	A	C2-N3-C4	18.71	119.95	110.60
1	AA	1374	A	N1-C6-N6	-18.71	107.38	118.60
22	BA	1014	A	N1-C6-N6	-18.71	107.38	118.60
22	BA	2433	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	382	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	918	A	C2-N3-C4	18.70	119.95	110.60
23	BB	45	A	C2-N3-C4	18.70	119.95	110.60
22	BA	10	A	C2-N3-C4	18.70	119.95	110.60
1	AA	253	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	1271	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1280	A	C2-N3-C4	18.70	119.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	309	A	N1-C2-N3	-18.70	119.95	129.30
55	B8	51	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1430	A	N1-C6-N6	-18.70	107.38	118.60
22	BA	896	A	C2-N3-C4	18.70	119.95	110.60
22	BA	896	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	1885	A	C2-N3-C4	18.70	119.95	110.60
22	BA	2425	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	2753	A	C2-N3-C4	18.70	119.95	110.60
22	BA	1080	A	C2-N3-C4	18.69	119.95	110.60
22	BA	1580	A	N1-C2-N3	-18.69	119.95	129.30
22	BA	1676	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	596	A	N1-C2-N3	-18.69	119.95	129.30
22	BA	1077	A	C2-N3-C4	18.69	119.94	110.60
22	BA	1439	A	C2-N3-C4	18.69	119.94	110.60
22	BA	2893	A	N1-C2-N3	-18.69	119.96	129.30
22	BA	2352	A	N1-C2-N3	-18.69	119.96	129.30
22	BA	479	A	C2-N3-C4	18.69	119.94	110.60
1	AA	1446	A	N1-C2-N3	-18.68	119.96	129.30
23	BB	94	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1101	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1531	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1276	A	C2-N3-C4	18.68	119.94	110.60
23	BB	57	A	N1-C2-N3	-18.68	119.96	129.30
54	B7	9	A	C2-N3-C4	18.68	119.94	110.60
22	BA	233	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1626	A	C2-N3-C4	18.68	119.94	110.60
22	BA	2741	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	2748	A	C2-N3-C4	18.68	119.94	110.60
1	AA	65	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	996	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1288	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	766	A	N1-C6-N6	-18.67	107.40	118.60
1	AA	825	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	1437	A	N1-C2-N3	-18.67	119.97	129.30
22	BA	244	A	C2-N3-C4	18.67	119.94	110.60
22	BA	1095	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	909	A	C2-N3-C4	18.67	119.94	110.60
22	BA	1029	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	321	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	1755	A	C2-N3-C4	18.66	119.93	110.60
1	AA	482	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	554	A	N1-C2-N3	-18.66	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	919	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1398	A	C2-N3-C4	18.66	119.93	110.60
22	BA	181	A	C2-N3-C4	18.66	119.93	110.60
22	BA	677	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	2169	A	C2-N3-C4	18.66	119.93	110.60
22	BA	346	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1987	A	N1-C6-N6	-18.66	107.40	118.60
55	B8	73	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1261	A	N1-C2-N3	-18.66	119.97	129.30
55	B8	66	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1251	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	197	A	N1-C6-N6	-18.66	107.41	118.60
1	AA	574	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1251	A	C2-N3-C4	18.65	119.93	110.60
22	BA	165	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	300	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	1762	A	C2-N3-C4	18.65	119.93	110.60
22	BA	2406	A	C2-N3-C4	18.65	119.93	110.60
22	BA	2734	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	155	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	44	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	2497	A	C2-N3-C4	18.65	119.92	110.60
22	BA	2725	A	C2-N3-C4	18.65	119.92	110.60
1	AA	205	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	889	A	C2-N3-C4	18.65	119.92	110.60
22	BA	721	A	C2-N3-C4	18.65	119.92	110.60
22	BA	1050	A	N1-C2-N3	-18.65	119.98	129.30
22	BA	793	A	C2-N3-C4	18.64	119.92	110.60
22	BA	1090	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	2860	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	68	G	N7-C8-N9	18.64	122.42	113.10
1	AA	560	A	C2-N3-C4	18.64	119.92	110.60
1	AA	938	A	C2-N3-C4	18.64	119.92	110.60
1	AA	1468	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	1502	A	C2-N3-C4	18.64	119.92	110.60
22	BA	1528	A	C2-N3-C4	18.64	119.92	110.60
23	BB	73	A	C2-N3-C4	18.64	119.92	110.60
1	AA	687	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	753	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	1392	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	2273	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	2317	A	N1-C6-N6	-18.64	107.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	630	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	6	A	C2-N3-C4	18.63	119.92	110.60
22	BA	125	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	1552	A	C2-N3-C4	18.63	119.92	110.60
22	BA	2560	A	N1-C2-N3	-18.63	119.98	129.30
55	B8	58	A	C2-N3-C4	18.63	119.92	110.60
1	AA	451	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	1396	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	1579	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	1746	A	C2-N3-C4	18.63	119.91	110.60
1	AA	109	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	675	A	C2-N3-C4	18.62	119.91	110.60
22	BA	1698	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	160	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	195	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	968	A	C2-N3-C4	18.62	119.91	110.60
22	BA	223	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	432	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	941	A	C2-N3-C4	18.62	119.91	110.60
1	AA	32	A	C2-N3-C4	18.62	119.91	110.60
1	AA	408	A	C2-N3-C4	18.62	119.91	110.60
1	AA	743	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	892	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	1785	A	C2-N3-C4	18.62	119.91	110.60
1	AA	253	A	C2-N3-C4	18.62	119.91	110.60
1	AA	964	A	C2-N3-C4	18.61	119.91	110.60
22	BA	2142	A	C2-N3-C4	18.61	119.91	110.60
1	AA	478	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	499	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	1306	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	2119	A	C2-N3-C4	18.61	119.91	110.60
1	AA	642	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	2547	A	C2-N3-C4	18.61	119.90	110.60
1	AA	236	A	N1-C2-N3	-18.61	120.00	129.30
55	B8	69	A	C2-N3-C4	18.61	119.90	110.60
1	AA	635	A	C2-N3-C4	18.60	119.90	110.60
22	BA	233	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	272	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	368	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	2459	A	C2-N3-C4	18.60	119.90	110.60
1	AA	172	A	C2-N3-C4	18.60	119.90	110.60
22	BA	2297	A	N1-C2-N3	-18.60	120.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1786	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	2411	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	408	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	125	A	C2-N3-C4	18.59	119.90	110.60
22	BA	382	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	1918	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	925	A	C2-N3-C4	18.59	119.90	110.60
22	BA	909	A	N1-C6-N6	-18.59	107.45	118.60
22	BA	2173	A	C2-N3-C4	18.59	119.89	110.60
1	AA	1363	A	N1-C6-N6	-18.59	107.45	118.60
22	BA	1084	A	C2-N3-C4	18.59	119.89	110.60
22	BA	94	A	C2-N3-C4	18.58	119.89	110.60
22	BA	1385	A	C2-N3-C4	18.58	119.89	110.60
22	BA	1803	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	71	A	C2-N3-C4	18.58	119.89	110.60
22	BA	146	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	616	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2810	A	C2-N3-C4	18.58	119.89	110.60
22	BA	1960	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2013	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2352	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	1375	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	52	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1142	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1532	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1528	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1690	A	C2-N3-C4	18.57	119.89	110.60
1	AA	1339	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	1048	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	2013	A	C2-N3-C4	18.57	119.89	110.60
1	AA	502	A	C2-N3-C4	18.57	119.88	110.60
1	AA	676	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	712	A	C2-N3-C4	18.57	119.89	110.60
1	AA	1476	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	2366	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	2882	A	C2-N3-C4	18.57	119.88	110.60
1	AA	1093	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1152	A	C2-N3-C4	18.57	119.88	110.60
22	BA	878	A	C2-N3-C4	18.57	119.88	110.60
22	BA	2014	A	C2-N3-C4	18.57	119.88	110.60
1	AA	393	A	C2-N3-C4	18.57	119.88	110.60
22	BA	705	A	N1-C2-N3	-18.57	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1495	A	C2-N3-C4	18.57	119.88	110.60
22	BA	2482	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	729	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	10	A	C2-N3-C4	18.56	119.88	110.60
1	AA	452	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	1329	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1188	A	C2-N3-C4	18.56	119.88	110.60
1	AA	143	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	149	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1287	A	N1-C6-N6	-18.56	107.47	118.60
22	BA	1151	A	N1-C6-N6	-18.56	107.47	118.60
22	BA	2887	A	C2-N3-C4	18.56	119.88	110.60
22	BA	1916	A	C2-N3-C4	18.55	119.88	110.60
22	BA	2530	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	119	A	C2-N3-C4	18.55	119.88	110.60
22	BA	501	A	C2-N3-C4	18.55	119.88	110.60
1	AA	913	A	C2-N3-C4	18.55	119.87	110.60
22	BA	592	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	1067	A	C2-N3-C4	18.55	119.87	110.60
22	BA	1496	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	878	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	716	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	2800	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1085	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1549	A	N1-C6-N6	-18.54	107.47	118.60
22	BA	125	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	53	A	C2-N3-C4	18.54	119.87	110.60
22	BA	2095	A	C2-N3-C4	18.54	119.87	110.60
1	AA	160	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	728	A	C2-N3-C4	18.54	119.87	110.60
22	BA	430	A	C2-N3-C4	18.54	119.87	110.60
1	AA	98	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1508	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1534	A	C2-N3-C4	18.53	119.87	110.60
1	AA	1346	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	2531	A	C2-N3-C4	18.53	119.87	110.60
22	BA	342	A	C2-N3-C4	18.53	119.86	110.60
22	BA	1321	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	1551	A	C2-N3-C4	18.53	119.86	110.60
1	AA	937	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	1147	A	N1-C2-N3	-18.53	120.04	129.30
22	BA	1268	A	N1-C6-N6	-18.53	107.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	205	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1280	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	2211	A	C2-N3-C4	18.52	119.86	110.60
1	AA	583	A	C2-N3-C4	18.52	119.86	110.60
1	AA	353	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	654	A	C2-N3-C4	18.52	119.86	110.60
22	BA	877	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	167	A	C2-N3-C4	18.52	119.86	110.60
22	BA	84	A	C2-N3-C4	18.52	119.86	110.60
22	BA	332	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	2425	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	460	A	C2-N3-C4	18.52	119.86	110.60
22	BA	172	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2126	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1899	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	236	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	968	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	1213	A	C2-N3-C4	18.51	119.86	110.60
22	BA	979	A	C2-N3-C4	18.51	119.86	110.60
22	BA	1952	A	C2-N3-C4	18.51	119.86	110.60
22	BA	6	A	N1-C2-N3	-18.51	120.04	129.30
22	BA	2426	A	C2-N3-C4	18.51	119.86	110.60
22	BA	936	A	C2-N3-C4	18.51	119.86	110.60
22	BA	172	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	560	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	574	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2060	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	2284	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1900	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	553	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	1102	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	203	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2183	A	C2-N3-C4	18.50	119.85	110.60
1	AA	1111	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	1429	A	C2-N3-C4	18.50	119.85	110.60
22	BA	182	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	1237	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1773	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	2734	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	706	A	C2-N3-C4	18.50	119.85	110.60
22	BA	706	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	554	A	C2-N3-C4	18.49	119.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1876	A	N1-C2-N3	-18.49	120.05	129.30
55	B8	38	A	N1-C2-N3	-18.49	120.05	129.30
1	AA	155	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	532	A	C2-N3-C4	18.49	119.84	110.60
22	BA	1566	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	309	A	C2-N3-C4	18.49	119.84	110.60
1	AA	320	A	C2-N3-C4	18.49	119.84	110.60
1	AA	1155	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	1456	A	C2-N3-C4	18.49	119.84	110.60
22	BA	1579	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	2015	A	C2-N3-C4	18.49	119.84	110.60
22	BA	2665	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	329	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	553	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	483	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	1241	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	162	A	C2-N3-C4	18.48	119.84	110.60
1	AA	288	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	382	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1689	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	1057	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	1264	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1916	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2813	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	478	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	975	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2199	A	C2-N3-C4	18.48	119.84	110.60
1	AA	161	A	C2-N3-C4	18.48	119.84	110.60
1	AA	559	A	N1-C6-N6	-18.48	107.52	118.60
22	BA	2163	A	N1-C6-N6	-18.48	107.52	118.60
1	AA	1306	A	C2-N3-C4	18.47	119.84	110.60
1	AA	72	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	1205	A	N1-C6-N6	-18.47	107.52	118.60
55	B8	14	A	N1-C2-N3	-18.47	120.06	129.30
23	BB	78	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	354	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	1453	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	1265	A	N1-C2-N3	-18.47	120.07	129.30
1	AA	80	A	C2-N3-C4	18.47	119.83	110.60
1	AA	1493	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	2837	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1328	A	C2-N3-C4	18.46	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1271	A	N1-C6-N6	-18.46	107.53	118.60
55	B8	42	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	441	A	C2-N3-C4	18.46	119.83	110.60
22	BA	352	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	649	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	538	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	590	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1089	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1307	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1853	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	681	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	2893	A	C2-N3-C4	18.45	119.83	110.60
23	BB	39	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	1289	A	C2-N3-C4	18.45	119.83	110.60
22	BA	371	A	C2-N3-C4	18.45	119.82	110.60
22	BA	1420	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	1453	A	C2-N3-C4	18.45	119.83	110.60
22	BA	2461	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	103	A	C2-N3-C4	18.45	119.82	110.60
22	BA	497	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	509	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	1531	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	1609	A	C2-N3-C4	18.45	119.82	110.60
22	BA	2412	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	1413	A	N1-C6-N6	-18.44	107.53	118.60
22	BA	2281	A	N1-C6-N6	-18.44	107.53	118.60
55	B8	76	A	C2-N3-C4	18.44	119.82	110.60
22	BA	131	A	C2-N3-C4	18.44	119.82	110.60
22	BA	391	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	21	A	N1-C6-N6	-18.44	107.54	118.60
22	BA	1265	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	1239	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	32	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	1004	A	C2-N3-C4	18.44	119.82	110.60
22	BA	896	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	815	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	1055	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	1447	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	704	A	N1-C6-N6	-18.43	107.55	118.60
22	BA	616	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	320	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2134	A	N1-C6-N6	-18.42	107.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2281	A	C2-N3-C4	18.42	119.81	110.60
1	AA	1170	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	64	A	N1-C6-N6	-18.42	107.55	118.60
22	BA	699	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2309	A	N1-C6-N6	-18.42	107.55	118.60
23	BB	108	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	197	A	C2-N3-C4	18.42	119.81	110.60
22	BA	1077	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	2899	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	1036	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2169	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	44	A	C2-N3-C4	18.42	119.81	110.60
1	AA	509	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	1499	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2170	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	1274	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	2173	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	2003	A	N1-C6-N6	-18.41	107.56	118.60
1	AA	1046	A	C2-N3-C4	18.41	119.80	110.60
1	AA	1145	A	C2-N3-C4	18.41	119.80	110.60
22	BA	574	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	715	A	C2-N3-C4	18.41	119.80	110.60
1	AA	702	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	1977	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	654	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	559	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	681	A	C2-N3-C4	18.40	119.80	110.60
1	AA	983	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	1349	A	C2-N3-C4	18.40	119.80	110.60
22	BA	1336	A	C2-N3-C4	18.40	119.80	110.60
55	B8	38	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2171	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2278	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	2381	A	C2-N3-C4	18.40	119.80	110.60
1	AA	596	A	C2-N3-C4	18.39	119.80	110.60
22	BA	218	A	C2-N3-C4	18.39	119.80	110.60
1	AA	389	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	592	A	C2-N3-C4	18.39	119.79	110.60
22	BA	1579	A	C2-N3-C4	18.39	119.80	110.60
22	BA	1780	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	1433	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	2134	A	N1-C2-N3	-18.39	120.11	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	52	A	C2-N3-C4	18.39	119.79	110.60
22	BA	1070	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	677	A	C2-N3-C4	18.38	119.79	110.60
1	AA	1269	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	1130	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	1596	A	C2-N3-C4	18.38	119.79	110.60
1	AA	1176	A	C2-N3-C4	18.38	119.79	110.60
1	AA	1248	A	C2-N3-C4	18.38	119.79	110.60
1	AA	1507	A	C2-N3-C4	18.38	119.79	110.60
22	BA	666	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	2761	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	2386	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	2600	A	N1-C6-N6	-18.38	107.58	118.60
22	BA	2654	A	N1-C2-N3	-18.37	120.11	129.30
55	B8	21	A	C2-N3-C4	18.37	119.79	110.60
1	AA	181	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	156	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	197	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	256	A	N1-C2-N3	-18.37	120.11	129.30
1	AA	649	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	784	A	N1-C2-N3	-18.37	120.12	129.30
22	BA	415	A	C2-N3-C4	18.37	119.78	110.60
1	AA	408	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	2191	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	1885	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1080	A	C2-N3-C4	18.36	119.78	110.60
1	AA	728	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1082	A	C2-N3-C4	18.36	119.78	110.60
23	BB	53	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	1288	A	C2-N3-C4	18.36	119.78	110.60
23	BB	119	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1067	A	N1-C2-N3	-18.35	120.12	129.30
22	BA	1801	A	C2-N3-C4	18.35	119.78	110.60
22	BA	2850	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	129	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	1428	A	C2-N3-C4	18.35	119.77	110.60
1	AA	1531	A	C2-N3-C4	18.35	119.77	110.60
22	BA	439	A	N1-C2-N3	-18.35	120.13	129.30
22	BA	2114	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	74	A	C2-N3-C4	18.34	119.77	110.60
1	AA	502	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	572	A	N1-C2-N3	-18.34	120.13	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	722	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	1794	A	N1-C6-N6	-18.34	107.59	118.60
1	AA	1004	A	N1-C6-N6	-18.34	107.60	118.60
22	BA	311	A	C2-N3-C4	18.34	119.77	110.60
22	BA	515	A	C2-N3-C4	18.34	119.77	110.60
22	BA	979	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	223	A	C2-N3-C4	18.34	119.77	110.60
22	BA	84	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	26	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	325	A	N1-C2-N3	-18.33	120.13	129.30
1	AA	1111	A	C2-N3-C4	18.33	119.77	110.60
22	BA	1353	A	N1-C2-N3	-18.33	120.13	129.30
1	AA	1374	A	C2-N3-C4	18.33	119.76	110.60
22	BA	348	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	1366	A	C2-N3-C4	18.33	119.77	110.60
1	AA	162	A	N1-C2-N3	-18.33	120.14	129.30
1	AA	1368	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	1810	A	C2-N3-C4	18.33	119.76	110.60
23	BB	45	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1408	A	N1-C2-N3	-18.33	120.14	129.30
1	AA	1012	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1092	A	C2-N3-C4	18.32	119.76	110.60
55	B8	26	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	95	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	2835	A	C2-N3-C4	18.32	119.76	110.60
1	AA	167	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	575	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2478	A	C2-N3-C4	18.32	119.76	110.60
55	B8	6	A	C2-N3-C4	18.32	119.76	110.60
1	AA	1377	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	2147	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2469	A	C2-N3-C4	18.32	119.76	110.60
22	BA	91	A	N1-C2-N3	-18.31	120.14	129.30
1	AA	1110	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	572	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	2821	A	C2-N3-C4	18.31	119.76	110.60
22	BA	1913	A	N1-C6-N6	-18.31	107.61	118.60
1	AA	80	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	340	A	N1-C6-N6	-18.31	107.61	118.60
22	BA	2170	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1327	A	C2-N3-C4	18.31	119.75	110.60
55	B8	41	A	N1-C6-N6	-18.31	107.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1394	A	C2-N3-C4	18.31	119.75	110.60
55	B8	59	A	C2-N3-C4	18.31	119.75	110.60
1	AA	510	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1274	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	270	A	C2-N3-C4	18.30	119.75	110.60
1	AA	1513	A	C2-N3-C4	18.30	119.75	110.60
22	BA	781	A	C2-N3-C4	18.30	119.75	110.60
1	AA	1503	A	C2-N3-C4	18.30	119.75	110.60
1	AA	28	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1494	A	C2-N3-C4	18.30	119.75	110.60
1	AA	415	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	914	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1735	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	663	A	C2-N3-C4	18.29	119.75	110.60
1	AA	1434	A	C2-N3-C4	18.29	119.75	110.60
22	BA	1494	A	N1-C6-N6	-18.29	107.62	118.60
22	BA	2589	A	N1-C6-N6	-18.29	107.62	118.60
1	AA	2	A	N1-C6-N6	-18.29	107.63	118.60
1	AA	171	A	N1-C2-N3	-18.29	120.15	129.30
22	BA	1070	A	C2-N3-C4	18.29	119.75	110.60
1	AA	349	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	515	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	1711	A	C2-N3-C4	18.29	119.74	110.60
22	BA	324	A	N1-C6-N6	-18.29	107.63	118.60
1	AA	389	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	609	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	563	A	N1-C2-N3	-18.28	120.16	129.30
1	AA	1170	A	C2-N3-C4	18.28	119.74	110.60
22	BA	217	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	1069	A	C2-N3-C4	18.28	119.74	110.60
1	AA	172	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	226	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	2459	A	N1-C2-N3	-18.28	120.16	129.30
1	AA	270	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	1367	A	C2-N3-C4	18.28	119.74	110.60
22	BA	2082	A	C2-N3-C4	18.28	119.74	110.60
1	AA	807	A	C2-N3-C4	18.28	119.74	110.60
1	AA	1155	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	1311	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	1744	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	1952	A	N1-C6-N6	-18.27	107.64	118.60
55	B8	73	A	C2-N3-C4	18.27	119.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1299	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	2547	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	55	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	513	A	C2-N3-C4	18.27	119.73	110.60
22	BA	63	A	C2-N3-C4	18.27	119.73	110.60
22	BA	1342	A	C2-N3-C4	18.27	119.73	110.60
22	BA	1495	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	2297	A	C2-N3-C4	18.26	119.73	110.60
1	AA	1360	A	C2-N3-C4	18.26	119.73	110.60
22	BA	191	A	C2-N3-C4	18.26	119.73	110.60
22	BA	1802	A	C2-N3-C4	18.26	119.73	110.60
22	BA	2734	A	C2-N3-C4	18.26	119.73	110.60
1	AA	1111	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	613	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	1284	A	C2-N3-C4	18.26	119.73	110.60
22	BA	1477	A	C2-N3-C4	18.26	119.73	110.60
23	BB	57	A	C2-N3-C4	18.26	119.73	110.60
22	BA	1439	A	N1-C6-N6	-18.26	107.65	118.60
1	AA	1012	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	362	A	C2-N3-C4	18.25	119.73	110.60
22	BA	900	A	C2-N3-C4	18.25	119.73	110.60
22	BA	1001	A	C2-N3-C4	18.25	119.73	110.60
22	BA	1847	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	766	A	C2-N3-C4	18.25	119.73	110.60
1	AA	371	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	907	A	C2-N3-C4	18.25	119.73	110.60
1	AA	819	A	N1-C6-N6	-18.25	107.65	118.60
55	B8	51	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	643	A	N1-C2-N3	-18.25	120.18	129.30
22	BA	2335	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	81	A	C2-N3-C4	18.25	119.72	110.60
22	BA	346	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	925	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	78	A	C2-N3-C4	18.24	119.72	110.60
22	BA	603	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	974	A	C2-N3-C4	18.24	119.72	110.60
1	AA	432	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	1469	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2430	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	2587	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2809	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	1586	A	C2-N3-C4	18.24	119.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	371	A	C2-N3-C4	18.23	119.72	110.60
1	AA	753	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	1084	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	2657	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	782	A	C2-N3-C4	18.23	119.71	110.60
1	AA	1067	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	428	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	1590	A	N1-C2-N3	-18.23	120.19	129.30
22	BA	2799	A	N1-C2-N3	-18.23	120.19	129.30
22	BA	988	A	C2-N3-C4	18.23	119.71	110.60
1	AA	373	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	1110	A	N1-C6-N6	-18.23	107.67	118.60
22	BA	2741	A	N1-C6-N6	-18.23	107.67	118.60
22	BA	152	A	C2-N3-C4	18.22	119.71	110.60
22	BA	1509	A	N1-C6-N6	-18.22	107.67	118.60
22	BA	1342	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	1483	A	C2-N3-C4	18.22	119.71	110.60
1	AA	33	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	1346	A	C2-N3-C4	18.22	119.71	110.60
22	BA	2369	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	1229	A	C2-N3-C4	18.21	119.71	110.60
1	AA	1363	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	1783	A	C2-N3-C4	18.21	119.71	110.60
22	BA	1912	A	N1-C2-N3	-18.21	120.19	129.30
1	AA	487	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	104	A	C2-N3-C4	18.21	119.71	110.60
1	AA	949	A	N1-C2-N3	-18.21	120.19	129.30
1	AA	781	A	C2-N3-C4	18.21	119.70	110.60
1	AA	190	A	C2-N3-C4	18.21	119.70	110.60
1	AA	642	A	C2-N3-C4	18.20	119.70	110.60
22	BA	1470	A	C2-N3-C4	18.20	119.70	110.60
22	BA	2518	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	635	A	N1-C6-N6	-18.20	107.68	118.60
55	B8	58	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	784	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	2461	A	N1-C6-N6	-18.20	107.68	118.60
23	BB	50	A	C2-N3-C4	18.20	119.70	110.60
1	AA	306	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	802	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	1257	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	478	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	1368	A	N1-C6-N6	-18.19	107.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	221	A	N1-C6-N6	-18.19	107.68	118.60
23	BB	109	A	C2-N3-C4	18.19	119.70	110.60
1	AA	411	A	C2-N3-C4	18.19	119.70	110.60
1	AA	915	A	C2-N3-C4	18.19	119.69	110.60
22	BA	706	A	N1-C6-N6	-18.19	107.69	118.60
1	AA	1169	A	N1-C2-N3	-18.19	120.21	129.30
22	BA	152	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	2572	A	N1-C2-N3	-18.19	120.21	129.30
1	AA	712	A	N1-C2-N3	-18.18	120.21	129.30
1	AA	1093	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	382	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	423	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2482	A	N1-C6-N6	-18.18	107.69	118.60
55	B8	6	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	582	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	716	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	1214	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	221	A	C2-N3-C4	18.18	119.69	110.60
22	BA	1711	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	1854	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2142	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	526	A	N1-C2-N3	-18.17	120.21	129.30
1	AA	706	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	1503	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	1928	A	C2-N3-C4	18.17	119.69	110.60
22	BA	2101	A	C2-N3-C4	18.17	119.69	110.60
22	BA	2776	A	C2-N3-C4	18.17	119.69	110.60
1	AA	767	A	C2-N3-C4	18.17	119.68	110.60
1	AA	459	A	N1-C2-N3	-18.17	120.22	129.30
23	BB	15	A	C2-N3-C4	18.17	119.68	110.60
22	BA	161	A	C2-N3-C4	18.17	119.68	110.60
22	BA	2336	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	2453	A	N1-C2-N3	-18.17	120.22	129.30
22	BA	2634	A	N1-C2-N3	-18.17	120.22	129.30
1	AA	298	A	C2-N3-C4	18.16	119.68	110.60
1	AA	303	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	621	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1735	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	173	A	C2-N3-C4	18.16	119.68	110.60
22	BA	1272	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	77	A	N1-C6-N6	-18.16	107.70	118.60
55	B8	66	A	N1-C6-N6	-18.16	107.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1591	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	66	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2095	A	N1-C2-N3	-18.16	120.22	129.30
1	AA	452	A	C2-N3-C4	18.16	119.68	110.60
1	AA	1285	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	167	A	N1-C2-N3	-18.15	120.22	129.30
55	B8	59	A	N1-C6-N6	-18.15	107.71	118.60
1	AA	1219	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	947	A	C2-N3-C4	18.15	119.67	110.60
22	BA	1353	A	C2-N3-C4	18.15	119.67	110.60
1	AA	199	A	C2-N3-C4	18.15	119.67	110.60
1	AA	466	A	N1-C2-N3	-18.15	120.23	129.30
22	BA	2860	A	C2-N3-C4	18.15	119.67	110.60
1	AA	1483	A	N1-C2-N3	-18.15	120.23	129.30
22	BA	149	A	C2-N3-C4	18.15	119.67	110.60
22	BA	2727	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	2792	A	C2-N3-C4	18.14	119.67	110.60
22	BA	204	A	C2-N3-C4	18.14	119.67	110.60
22	BA	1088	A	N1-C6-N6	-18.14	107.71	118.60
22	BA	1739	A	C2-N3-C4	18.14	119.67	110.60
22	BA	2184	A	N1-C2-N3	-18.14	120.23	129.30
1	AA	510	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	5	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1020	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	1304	A	N1-C2-N3	-18.14	120.23	129.30
1	AA	196	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	1150	A	C2-N3-C4	18.14	119.67	110.60
1	AA	1429	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	526	A	C2-N3-C4	18.14	119.67	110.60
22	BA	2225	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	2378	A	C2-N3-C4	18.14	119.67	110.60
22	BA	2097	A	N1-C2-N3	-18.14	120.23	129.30
1	AA	1191	A	C2-N3-C4	18.13	119.67	110.60
1	AA	790	A	C2-N3-C4	18.13	119.67	110.60
22	BA	1143	A	C2-N3-C4	18.13	119.67	110.60
22	BA	1276	A	N1-C6-N6	-18.13	107.72	118.60
23	BB	58	A	N1-C2-N3	-18.13	120.23	129.30
22	BA	547	A	N1-C2-N3	-18.13	120.23	129.30
1	AA	171	A	C2-N3-C4	18.13	119.67	110.60
1	AA	502	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	1176	A	N1-C2-N3	-18.13	120.23	129.30
1	AA	465	A	N1-C6-N6	-18.13	107.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	814	A	C2-N3-C4	18.13	119.66	110.60
22	BA	2376	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	831	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	1306	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	101	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	831	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	1430	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	1791	A	C2-N3-C4	18.12	119.66	110.60
22	BA	1020	A	C2-N3-C4	18.12	119.66	110.60
1	AA	640	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	663	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	831	A	C2-N3-C4	18.12	119.66	110.60
22	BA	2198	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	602	A	N1-C6-N6	-18.11	107.73	118.60
22	BA	19	A	C2-N3-C4	18.11	119.66	110.60
1	AA	33	A	C2-N3-C4	18.11	119.66	110.60
1	AA	609	A	C2-N3-C4	18.11	119.66	110.60
1	AA	753	A	C2-N3-C4	18.11	119.66	110.60
22	BA	324	A	C2-N3-C4	18.11	119.66	110.60
22	BA	563	A	C2-N3-C4	18.11	119.65	110.60
1	AA	223	A	N1-C2-N3	-18.11	120.25	129.30
1	AA	1502	A	N1-C6-N6	-18.11	107.74	118.60
22	BA	1084	A	N1-C6-N6	-18.11	107.74	118.60
1	AA	878	A	N1-C2-N3	-18.10	120.25	129.30
1	AA	1493	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	1583	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	1634	A	C2-N3-C4	18.10	119.65	110.60
55	B8	69	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	2448	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	429	A	C2-N3-C4	18.10	119.65	110.60
1	AA	1019	A	C2-N3-C4	18.10	119.65	110.60
22	BA	374	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	1553	A	C2-N3-C4	18.10	119.65	110.60
22	BA	899	A	C2-N3-C4	18.09	119.65	110.60
22	BA	1226	A	N1-C6-N6	-18.09	107.74	118.60
1	AA	1324	A	N1-C2-N3	-18.09	120.25	129.30
22	BA	655	A	N1-C6-N6	-18.09	107.74	118.60
1	AA	250	A	C2-N3-C4	18.09	119.64	110.60
22	BA	2657	A	C2-N3-C4	18.09	119.64	110.60
1	AA	1508	A	N1-C2-N3	-18.09	120.26	129.30
22	BA	983	A	C2-N3-C4	18.09	119.64	110.60
22	BA	2598	A	N1-C2-N3	-18.09	120.25	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	279	A	N1-C2-N3	-18.09	120.26	129.30
1	AA	313	A	N1-C2-N3	-18.09	120.26	129.30
1	AA	777	A	C2-N3-C4	18.09	119.64	110.60
22	BA	1230	A	N1-C6-N6	-18.09	107.75	118.60
23	BB	46	A	C2-N3-C4	18.09	119.64	110.60
1	AA	602	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	2198	A	C2-N3-C4	18.08	119.64	110.60
22	BA	2184	A	C2-N3-C4	18.08	119.64	110.60
1	AA	1004	A	N1-C2-N3	-18.08	120.26	129.30
22	BA	1021	A	N1-C2-N3	-18.08	120.26	129.30
22	BA	2850	A	C2-N3-C4	18.08	119.64	110.60
1	AA	807	A	N1-C2-N3	-18.07	120.26	129.30
22	BA	735	A	C2-N3-C4	18.07	119.64	110.60
22	BA	727	A	C2-N3-C4	18.07	119.64	110.60
1	AA	1092	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	354	A	C2-N3-C4	18.07	119.64	110.60
22	BA	207	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	2820	A	C2-N3-C4	18.07	119.63	110.60
22	BA	2336	A	C2-N3-C4	18.06	119.63	110.60
22	BA	161	A	N1-C6-N6	-18.06	107.76	118.60
22	BA	1169	A	N1-C6-N6	-18.06	107.76	118.60
1	AA	329	A	C2-N3-C4	18.06	119.63	110.60
22	BA	71	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	2284	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	663	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	1005	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	665	A	C2-N3-C4	18.05	119.62	110.60
22	BA	1918	A	C2-N3-C4	18.05	119.62	110.60
22	BA	2340	A	C2-N3-C4	18.05	119.62	110.60
22	BA	1230	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	42	A	C2-N3-C4	18.05	119.62	110.60
22	BA	794	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	1359	A	C2-N3-C4	18.05	119.62	110.60
22	BA	1919	A	C2-N3-C4	18.05	119.62	110.60
1	AA	78	A	N1-C6-N6	-18.04	107.77	118.60
22	BA	1260	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	945	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	1254	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	1447	A	C2-N3-C4	18.04	119.62	110.60
22	BA	204	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	2765	A	N1-C6-N6	-18.04	107.78	118.60
1	AA	596	A	N1-C6-N6	-18.03	107.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	937	A	N1-C2-N3	-18.03	120.28	129.30
1	AA	1431	A	C2-N3-C4	18.03	119.62	110.60
22	BA	1054	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	1509	A	C2-N3-C4	18.03	119.62	110.60
22	BA	2191	A	N1-C2-N3	-18.03	120.28	129.30
1	AA	1408	A	C2-N3-C4	18.03	119.61	110.60
1	AA	974	A	N1-C6-N6	-18.03	107.78	118.60
1	AA	1254	A	C2-N3-C4	18.03	119.61	110.60
22	BA	685	A	N1-C6-N6	-18.03	107.78	118.60
22	BA	2471	A	C2-N3-C4	18.03	119.61	110.60
22	BA	278	A	C2-N3-C4	18.03	119.61	110.60
1	AA	1082	A	N1-C6-N6	-18.02	107.79	118.60
23	BB	46	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	472	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	1318	A	C2-N3-C4	18.02	119.61	110.60
1	AA	430	A	C2-N3-C4	18.02	119.61	110.60
1	AA	495	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	1350	A	C2-N3-C4	18.02	119.61	110.60
22	BA	279	A	N1-C2-N3	-18.02	120.29	129.30
1	AA	487	A	C2-N3-C4	18.02	119.61	110.60
1	AA	1167	A	C2-N3-C4	18.02	119.61	110.60
22	BA	492	A	N1-C2-N3	-18.01	120.29	129.30
1	AA	179	A	N1-C2-N3	-18.01	120.30	129.30
1	AA	1324	A	C2-N3-C4	18.01	119.61	110.60
22	BA	1048	A	C2-N3-C4	18.01	119.61	110.60
1	AA	1350	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	1197	A	C2-N3-C4	18.00	119.60	110.60
22	BA	2736	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	533	A	C2-N3-C4	17.99	119.60	110.60
1	AA	1204	A	C2-N3-C4	17.99	119.60	110.60
22	BA	844	A	N1-C2-N3	-17.99	120.30	129.30
22	BA	2183	A	N1-C2-N3	-17.99	120.30	129.30
1	AA	1257	A	N1-C2-N3	-17.99	120.31	129.30
22	BA	127	A	N1-C2-N3	-17.99	120.31	129.30
22	BA	863	A	C2-N3-C4	17.99	119.59	110.60
22	BA	401	A	C2-N3-C4	17.99	119.59	110.60
22	BA	2108	A	C2-N3-C4	17.99	119.59	110.60
1	AA	1238	A	C2-N3-C4	17.98	119.59	110.60
22	BA	936	A	N1-C6-N6	-17.98	107.81	118.60
1	AA	1374	A	N1-C2-N3	-17.98	120.31	129.30
1	AA	901	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	781	A	N1-C2-N3	-17.98	120.31	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1570	A	N1-C6-N6	-17.98	107.81	118.60
1	AA	1130	A	C2-N3-C4	17.98	119.59	110.60
22	BA	1700	A	C2-N3-C4	17.98	119.59	110.60
1	AA	1130	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	362	A	N1-C2-N3	-17.97	120.31	129.30
1	AA	116	A	C2-N3-C4	17.97	119.58	110.60
22	BA	2358	A	C2-N3-C4	17.97	119.58	110.60
1	AA	523	A	C2-N3-C4	17.97	119.58	110.60
22	BA	2199	A	N1-C6-N6	-17.96	107.82	118.60
22	BA	2738	A	C2-N3-C4	17.96	119.58	110.60
1	AA	74	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	553	A	C2-N3-C4	17.96	119.58	110.60
1	AA	673	A	N1-C6-N6	-17.96	107.83	118.60
1	AA	949	A	N1-C6-N6	-17.96	107.83	118.60
22	BA	1080	A	N1-C6-N6	-17.96	107.83	118.60
22	BA	251	A	C2-N3-C4	17.96	119.58	110.60
1	AA	33	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	155	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	1086	A	C2-N3-C4	17.95	119.58	110.60
22	BA	2899	A	C2-N3-C4	17.95	119.58	110.60
1	AA	978	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	167	A	C2-N3-C4	17.95	119.58	110.60
22	BA	503	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	391	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1230	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1858	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1496	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1953	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	1754	A	C2-N3-C4	17.94	119.57	110.60
1	AA	1014	A	N1-C6-N6	-17.94	107.84	118.60
1	AA	1350	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	21	A	C2-N3-C4	17.94	119.57	110.60
22	BA	2799	A	C2-N3-C4	17.94	119.57	110.60
1	AA	978	A	C2-N3-C4	17.94	119.57	110.60
1	AA	1287	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	1522	A	C2-N3-C4	17.94	119.57	110.60
22	BA	447	A	C2-N3-C4	17.94	119.57	110.60
22	BA	156	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	1366	A	N1-C6-N6	-17.94	107.84	118.60
1	AA	3	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	1274	A	C2-N3-C4	17.93	119.57	110.60
22	BA	2094	A	N1-C6-N6	-17.93	107.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1609	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	1336	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	2468	A	C2-N3-C4	17.93	119.57	110.60
1	AA	1021	A	C2-N3-C4	17.93	119.56	110.60
22	BA	443	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	621	A	C2-N3-C4	17.93	119.56	110.60
22	BA	1247	A	N1-C2-N3	-17.93	120.34	129.30
22	BA	541	A	C2-N3-C4	17.93	119.56	110.60
22	BA	2147	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	129	A	C2-N3-C4	17.92	119.56	110.60
1	AA	901	A	C2-N3-C4	17.92	119.56	110.60
1	AA	794	A	C2-N3-C4	17.92	119.56	110.60
1	AA	1093	A	C2-N3-C4	17.92	119.56	110.60
22	BA	2059	A	C2-N3-C4	17.92	119.56	110.60
22	BA	705	A	C2-N3-C4	17.91	119.55	110.60
22	BA	918	A	N1-C6-N6	-17.91	107.86	118.60
22	BA	5	A	C2-N3-C4	17.90	119.55	110.60
1	AA	1318	A	N1-C6-N6	-17.90	107.86	118.60
22	BA	2748	A	N1-C6-N6	-17.90	107.86	118.60
1	AA	959	A	N1-C6-N6	-17.90	107.86	118.60
1	AA	1238	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	1269	A	C2-N3-C4	17.90	119.55	110.60
22	BA	340	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	687	A	C2-N3-C4	17.89	119.55	110.60
1	AA	1216	A	C2-N3-C4	17.89	119.55	110.60
22	BA	165	A	C2-N3-C4	17.89	119.55	110.60
22	BA	1722	A	N1-C2-N3	-17.89	120.35	129.30
22	BA	218	A	N1-C6-N6	-17.89	107.87	118.60
1	AA	649	A	C2-N3-C4	17.89	119.54	110.60
22	BA	2386	A	N1-C6-N6	-17.89	107.87	118.60
22	BA	1566	A	C2-N3-C4	17.89	119.54	110.60
22	BA	340	A	C2-N3-C4	17.89	119.54	110.60
22	BA	1169	A	C2-N3-C4	17.89	119.54	110.60
22	BA	1286	A	N1-C6-N6	-17.88	107.87	118.60
22	BA	1367	A	N1-C6-N6	-17.88	107.87	118.60
1	AA	1021	A	N1-C6-N6	-17.88	107.87	118.60
1	AA	1285	A	C2-N3-C4	17.88	119.54	110.60
22	BA	505	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	2298	A	C2-N3-C4	17.88	119.54	110.60
22	BA	2059	A	N1-C2-N3	-17.88	120.36	129.30
1	AA	1250	A	C2-N3-C4	17.87	119.54	110.60
22	BA	49	A	N1-C6-N6	-17.87	107.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1254	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	2211	A	N1-C6-N6	-17.87	107.88	118.60
1	AA	44	A	N1-C2-N3	-17.87	120.36	129.30
1	AA	642	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	2311	A	N1-C2-N3	-17.87	120.36	129.30
1	AA	1067	A	C2-N3-C4	17.87	119.53	110.60
1	AA	432	A	C2-N3-C4	17.87	119.53	110.60
1	AA	629	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	715	A	C2-N3-C4	17.86	119.53	110.60
22	BA	2439	A	C2-N3-C4	17.86	119.53	110.60
1	AA	579	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1057	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	81	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	573	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	629	A	C2-N3-C4	17.86	119.53	110.60
22	BA	146	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	2407	A	C2-N3-C4	17.86	119.53	110.60
22	BA	2433	A	C2-N3-C4	17.86	119.53	110.60
22	BA	2738	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	2758	A	N1-C6-N6	-17.86	107.88	118.60
22	BA	1383	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	804	A	C2-N3-C4	17.86	119.53	110.60
22	BA	735	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	430	A	N1-C2-N3	-17.85	120.37	129.30
22	BA	1144	A	C2-N3-C4	17.85	119.53	110.60
22	BA	2660	A	C2-N3-C4	17.85	119.53	110.60
22	BA	1545	A	C2-N3-C4	17.85	119.52	110.60
22	BA	1801	A	N1-C6-N6	-17.85	107.89	118.60
1	AA	482	A	C2-N3-C4	17.84	119.52	110.60
22	BA	347	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1073	A	C2-N3-C4	17.84	119.52	110.60
22	BA	2887	A	N1-C6-N6	-17.84	107.89	118.60
1	AA	495	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	721	A	N1-C6-N6	-17.84	107.89	118.60
22	BA	1275	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	352	A	C2-N3-C4	17.84	119.52	110.60
22	BA	1794	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	2377	A	C2-N3-C4	17.84	119.52	110.60
1	AA	448	A	N1-C6-N6	-17.84	107.90	118.60
22	BA	1553	A	N1-C6-N6	-17.84	107.90	118.60
1	AA	673	A	N1-C2-N3	-17.83	120.38	129.30
22	BA	614	A	C2-N3-C4	17.83	119.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	676	A	C2-N3-C4	17.83	119.52	110.60
22	BA	1791	A	N1-C6-N6	-17.83	107.90	118.60
1	AA	743	A	C2-N3-C4	17.83	119.51	110.60
1	AA	781	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	2758	A	C2-N3-C4	17.83	119.51	110.60
22	BA	1847	A	C2-N3-C4	17.82	119.51	110.60
22	BA	251	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1378	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2412	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2176	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2893	A	N1-C6-N6	-17.82	107.91	118.60
1	AA	1082	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1503	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	344	A	C2-N3-C4	17.81	119.51	110.60
22	BA	2274	A	C2-N3-C4	17.81	119.51	110.60
1	AA	1456	A	N1-C6-N6	-17.81	107.91	118.60
22	BA	2019	A	N1-C6-N6	-17.81	107.91	118.60
22	BA	609	A	N1-C2-N3	-17.81	120.40	129.30
22	BA	2009	A	N1-C6-N6	-17.80	107.92	118.60
1	AA	1468	A	C2-N3-C4	17.80	119.50	110.60
22	BA	73	A	C2-N3-C4	17.80	119.50	110.60
22	BA	149	A	N1-C2-N3	-17.80	120.40	129.30
1	AA	131	A	N1-C6-N6	-17.80	107.92	118.60
1	AA	461	A	C2-N3-C4	17.80	119.50	110.60
22	BA	1610	A	N1-C6-N6	-17.80	107.92	118.60
22	BA	844	A	N1-C6-N6	-17.80	107.92	118.60
22	BA	2134	A	C2-N3-C4	17.80	119.50	110.60
1	AA	228	A	C2-N3-C4	17.79	119.50	110.60
1	AA	1180	A	N1-C6-N6	-17.79	107.92	118.60
22	BA	2317	A	N1-C2-N3	-17.79	120.40	129.30
22	BA	829	A	N1-C2-N3	-17.79	120.41	129.30
1	AA	246	A	N1-C6-N6	-17.79	107.93	118.60
23	BB	29	A	C2-N3-C4	17.79	119.49	110.60
22	BA	2352	A	C2-N3-C4	17.79	119.49	110.60
1	AA	414	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	2241	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	2670	A	N1-C2-N3	-17.78	120.41	129.30
23	BB	119	A	C2-N3-C4	17.78	119.49	110.60
1	AA	393	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	504	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	959	A	C2-N3-C4	17.78	119.49	110.60
22	BA	1413	A	N1-C6-N6	-17.78	107.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	415	A	C2-N3-C4	17.77	119.49	110.60
22	BA	2071	A	N1-C6-N6	-17.77	107.94	118.60
1	AA	1105	A	C2-N3-C4	17.77	119.49	110.60
22	BA	2114	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	2090	A	N1-C2-N3	-17.77	120.42	129.30
1	AA	435	A	N1-C6-N6	-17.77	107.94	118.60
1	AA	923	A	C2-N3-C4	17.77	119.48	110.60
22	BA	144	A	N1-C6-N6	-17.76	107.94	118.60
22	BA	2412	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	55	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	1981	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	749	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	384	A	C2-N3-C4	17.76	119.48	110.60
1	AA	1216	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	1227	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	1257	A	C2-N3-C4	17.76	119.48	110.60
22	BA	613	A	C2-N3-C4	17.76	119.48	110.60
22	BA	644	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	2346	A	N1-C2-N3	-17.75	120.42	129.30
1	AA	878	A	C2-N3-C4	17.75	119.48	110.60
1	AA	1508	A	C2-N3-C4	17.75	119.48	110.60
22	BA	925	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1655	A	C2-N3-C4	17.75	119.47	110.60
1	AA	1239	A	C2-N3-C4	17.75	119.47	110.60
1	AA	120	A	C2-N3-C4	17.75	119.47	110.60
22	BA	2322	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	272	A	N1-C6-N6	-17.74	107.95	118.60
1	AA	873	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2531	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	1394	A	N1-C6-N6	-17.74	107.96	118.60
1	AA	1227	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	1	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	873	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	1196	A	N1-C6-N6	-17.74	107.96	118.60
22	BA	1014	A	C2-N3-C4	17.74	119.47	110.60
22	BA	1689	A	C2-N3-C4	17.73	119.47	110.60
1	AA	1171	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	749	A	N1-C6-N6	-17.73	107.96	118.60
1	AA	1238	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	1960	A	C2-N3-C4	17.73	119.46	110.60
22	BA	2660	A	N1-C2-N3	-17.73	120.44	129.30
1	AA	1368	A	C2-N3-C4	17.72	119.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	227	A	C2-N3-C4	17.72	119.46	110.60
22	BA	1014	A	N1-C2-N3	-17.72	120.44	129.30
1	AA	913	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	2309	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	2705	A	N1-C6-N6	-17.72	107.97	118.60
1	AA	782	A	N1-C6-N6	-17.71	107.97	118.60
1	AA	865	A	N1-C2-N3	-17.71	120.44	129.30
22	BA	2266	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	2388	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	483	A	C2-N3-C4	17.71	119.45	110.60
1	AA	996	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	1787	A	C2-N3-C4	17.71	119.45	110.60
1	AA	1204	A	N1-C2-N3	-17.71	120.45	129.30
22	BA	1304	A	C2-N3-C4	17.71	119.45	110.60
22	BA	1403	A	N1-C2-N3	-17.71	120.45	129.30
22	BA	1508	A	C2-N3-C4	17.71	119.45	110.60
22	BA	980	A	C2-N3-C4	17.70	119.45	110.60
1	AA	728	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	2407	A	N1-C2-N3	-17.70	120.45	129.30
1	AA	1151	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	781	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	2052	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	492	A	C2-N3-C4	17.69	119.45	110.60
22	BA	508	A	N1-C6-N6	-17.69	107.98	118.60
22	BA	1872	A	C2-N3-C4	17.69	119.45	110.60
22	BA	2872	A	C5-C6-N6	17.69	137.85	123.70
22	BA	1590	A	N1-C6-N6	-17.69	107.99	118.60
1	AA	72	A	C2-N3-C4	17.69	119.44	110.60
1	AA	1434	A	N1-C6-N6	-17.69	107.99	118.60
55	B8	59	A	N1-C2-N3	-17.69	120.46	129.30
1	AA	238	A	C2-N3-C4	17.68	119.44	110.60
1	AA	1196	A	C2-N3-C4	17.68	119.44	110.60
1	AA	238	A	N1-C6-N6	-17.68	108.00	118.60
1	AA	938	A	N1-C6-N6	-17.68	107.99	118.60
22	BA	756	A	N1-C6-N6	-17.68	108.00	118.60
1	AA	298	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	19	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	432	A	C2-N3-C4	17.67	119.44	110.60
1	AA	53	A	N1-C2-N3	-17.67	120.47	129.30
22	BA	1757	A	C2-N3-C4	17.67	119.43	110.60
1	AA	718	A	C2-N3-C4	17.67	119.43	110.60
1	AA	1000	A	N1-C6-N6	-17.66	108.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	115	A	N1-C2-N3	-17.66	120.47	129.30
1	AA	1055	A	C2-N3-C4	17.66	119.43	110.60
22	BA	863	A	N1-C6-N6	-17.66	108.01	118.60
22	BA	1048	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1269	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1899	A	N1-C6-N6	-17.66	108.01	118.60
22	BA	2163	A	C2-N3-C4	17.66	119.43	110.60
22	BA	2309	A	C2-N3-C4	17.66	119.43	110.60
22	BA	2572	A	C2-N3-C4	17.65	119.43	110.60
22	BA	95	A	C2-N3-C4	17.65	119.42	110.60
22	BA	1637	A	N1-C6-N6	-17.65	108.01	118.60
22	BA	1746	A	N1-C2-N3	-17.65	120.47	129.30
22	BA	2837	A	N1-C6-N6	-17.65	108.01	118.60
22	BA	2679	A	N1-C2-N3	-17.65	120.48	129.30
22	BA	2851	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	643	A	C2-N3-C4	17.63	119.42	110.60
22	BA	1551	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	2662	A	N1-C2-N3	-17.63	120.48	129.30
1	AA	535	A	C2-N3-C4	17.63	119.42	110.60
1	AA	749	A	C2-N3-C4	17.63	119.42	110.60
1	AA	1408	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	572	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	861	A	N1-C6-N6	-17.63	108.02	118.60
1	AA	629	A	N1-C6-N6	-17.63	108.02	118.60
1	AA	718	A	N1-C2-N3	-17.63	120.49	129.30
1	AA	946	A	N1-C6-N6	-17.62	108.03	118.60
22	BA	2634	A	C2-N3-C4	17.62	119.41	110.60
22	BA	344	A	N1-C6-N6	-17.62	108.03	118.60
22	BA	480	A	N1-C6-N6	-17.62	108.03	118.60
1	AA	640	A	C2-N3-C4	17.62	119.41	110.60
22	BA	1551	A	N1-C2-N3	-17.61	120.49	129.30
22	BA	2531	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	460	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	10	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	2740	A	C2-N3-C4	17.61	119.41	110.60
1	AA	655	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	996	A	C2-N3-C4	17.60	119.40	110.60
22	BA	320	A	N1-C6-N6	-17.59	108.04	118.60
22	BA	1787	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	2205	A	N1-C2-N3	-17.59	120.50	129.30
1	AA	374	A	N1-C6-N6	-17.59	108.05	118.60
1	AA	493	A	N1-C6-N6	-17.59	108.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2453	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	348	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	2346	A	C2-N3-C4	17.59	119.39	110.60
1	AA	1157	A	N1-C2-N3	-17.58	120.51	129.30
22	BA	453	A	C2-N3-C4	17.58	119.39	110.60
22	BA	1046	A	C2-N3-C4	17.58	119.39	110.60
22	BA	2328	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	666	A	C2-N3-C4	17.58	119.39	110.60
1	AA	1225	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	309	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	2530	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2670	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2740	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	2335	A	C2-N3-C4	17.57	119.39	110.60
22	BA	342	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	849	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	1960	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	2482	A	C2-N3-C4	17.57	119.39	110.60
22	BA	207	A	C2-N3-C4	17.57	119.38	110.60
22	BA	761	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	1808	A	N1-C2-N3	-17.57	120.52	129.30
1	AA	968	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	368	A	C2-N3-C4	17.56	119.38	110.60
22	BA	1953	A	N1-C6-N6	-17.56	108.06	118.60
22	BA	2750	A	C2-N3-C4	17.56	119.38	110.60
1	AA	640	A	N1-C6-N6	-17.56	108.07	118.60
1	AA	1339	A	N1-C6-N6	-17.56	108.07	118.60
22	BA	28	A	N1-C6-N6	-17.56	108.07	118.60
1	AA	860	A	C2-N3-C4	17.55	119.38	110.60
22	BA	2268	A	N1-C2-N3	-17.55	120.52	129.30
22	BA	2886	A	C2-N3-C4	17.55	119.38	110.60
1	AA	860	A	N1-C2-N3	-17.55	120.52	129.30
22	BA	574	A	N1-C6-N6	-17.55	108.07	118.60
1	AA	51	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	2705	A	N1-C2-N3	-17.55	120.53	129.30
22	BA	1634	A	N1-C6-N6	-17.55	108.07	118.60
1	AA	139	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	644	A	N1-C2-N3	-17.55	120.53	129.30
22	BA	2541	A	C2-N3-C4	17.55	119.37	110.60
22	BA	1805	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	609	A	C2-N3-C4	17.54	119.37	110.60
22	BA	633	A	C2-N3-C4	17.54	119.37	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1169	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	2792	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1077	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	2850	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	899	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	1433	A	C2-N3-C4	17.54	119.37	110.60
23	BB	115	A	C2-N3-C4	17.53	119.36	110.60
22	BA	2015	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	104	A	N1-C2-N3	-17.53	120.54	129.30
22	BA	990	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	1677	A	N1-C6-N6	-17.52	108.08	118.60
1	AA	937	A	C2-N3-C4	17.52	119.36	110.60
1	AA	1275	A	N1-C6-N6	-17.52	108.09	118.60
22	BA	626	A	C2-N3-C4	17.52	119.36	110.60
22	BA	2101	A	N1-C6-N6	-17.52	108.09	118.60
22	BA	1073	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	1433	A	N1-C6-N6	-17.51	108.09	118.60
1	AA	533	A	N1-C6-N6	-17.51	108.09	118.60
1	AA	1110	A	C2-N3-C4	17.51	119.35	110.60
1	AA	1375	A	N1-C6-N6	-17.50	108.10	118.60
1	AA	1163	A	C2-N3-C4	17.50	119.35	110.60
22	BA	981	A	C2-N3-C4	17.50	119.35	110.60
1	AA	1201	A	C2-N3-C4	17.50	119.35	110.60
22	BA	947	A	N1-C6-N6	-17.49	108.10	118.60
22	BA	1953	A	C2-N3-C4	17.49	119.35	110.60
22	BA	223	A	C2-N3-C4	17.49	119.35	110.60
1	AA	712	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	21	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	2733	A	C2-N3-C4	17.49	119.34	110.60
1	AA	349	A	C2-N3-C4	17.48	119.34	110.60
22	BA	2171	A	N1-C6-N6	-17.48	108.11	118.60
54	B7	9	A	N1-C2-N3	-17.48	120.56	129.30
1	AA	1152	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	354	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	374	A	C2-N3-C4	17.48	119.34	110.60
22	BA	2278	A	C2-N3-C4	17.48	119.34	110.60
1	AA	468	A	C2-N3-C4	17.47	119.34	110.60
22	BA	614	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	1858	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	2577	A	N1-C6-N6	-17.47	108.12	118.60
1	AA	53	A	N1-C6-N6	-17.47	108.12	118.60
1	AA	288	A	N1-C2-N3	-17.47	120.57	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	432	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	782	A	N1-C6-N6	-17.46	108.12	118.60
22	BA	1616	A	C2-N3-C4	17.46	119.33	110.60
1	AA	1502	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	1745	A	C2-N3-C4	17.46	119.33	110.60
1	AA	749	A	N1-C6-N6	-17.45	108.13	118.60
1	AA	969	A	N1-C6-N6	-17.45	108.13	118.60
1	AA	860	A	N1-C6-N6	-17.45	108.13	118.60
1	AA	1274	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	1103	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	2287	A	C2-N3-C4	17.45	119.32	110.60
1	AA	270	A	N1-C6-N6	-17.45	108.13	118.60
23	BB	34	A	C2-N3-C4	17.44	119.32	110.60
22	BA	900	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	2225	A	C2-N3-C4	17.44	119.32	110.60
1	AA	415	A	N1-C6-N6	-17.44	108.14	118.60
1	AA	482	A	N1-C6-N6	-17.44	108.14	118.60
1	AA	914	A	C2-N3-C4	17.44	119.32	110.60
22	BA	716	A	C2-N3-C4	17.44	119.32	110.60
22	BA	460	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	1127	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	1532	A	C2-N3-C4	17.43	119.32	110.60
1	AA	1146	A	C2-N3-C4	17.43	119.31	110.60
22	BA	2054	A	N1-C2-N3	-17.43	120.59	129.30
1	AA	1299	A	C2-N3-C4	17.43	119.31	110.60
1	AA	353	A	C2-N3-C4	17.43	119.31	110.60
1	AA	192	A	N1-C6-N6	-17.42	108.15	118.60
1	AA	845	A	N1-C2-N3	-17.42	120.59	129.30
1	AA	130	A	C2-N3-C4	17.42	119.31	110.60
22	BA	761	A	N1-C6-N6	-17.42	108.15	118.60
55	B8	26	A	N1-C2-N3	-17.42	120.59	129.30
1	AA	1019	A	N1-C2-N3	-17.41	120.59	129.30
22	BA	541	A	N1-C6-N6	-17.41	108.15	118.60
1	AA	1169	A	C2-N3-C4	17.41	119.31	110.60
1	AA	1430	A	C2-N3-C4	17.41	119.31	110.60
1	AA	780	A	N1-C6-N6	-17.41	108.16	118.60
22	BA	2126	A	N1-C6-N6	-17.41	108.15	118.60
1	AA	151	A	N1-C2-N3	-17.41	120.60	129.30
1	AA	182	A	N1-C6-N6	-17.41	108.16	118.60
23	BB	78	A	C2-N3-C4	17.41	119.30	110.60
1	AA	702	A	N1-C6-N6	-17.40	108.16	118.60
22	BA	256	A	C2-N3-C4	17.40	119.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	493	A	C2-N3-C4	17.40	119.30	110.60
22	BA	734	A	C2-N3-C4	17.39	119.30	110.60
1	AA	747	A	N1-C2-N3	-17.39	120.60	129.30
1	AA	495	A	C2-N3-C4	17.39	119.29	110.60
1	AA	499	A	N1-C6-N6	-17.39	108.17	118.60
22	BA	255	A	N1-C2-N3	-17.39	120.61	129.30
22	BA	752	A	C5-C6-N6	17.39	137.61	123.70
22	BA	2322	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	2700	A	C2-N3-C4	17.38	119.29	110.60
22	BA	1427	A	C2-N3-C4	17.37	119.29	110.60
22	BA	1477	A	N1-C6-N6	-17.37	108.17	118.60
22	BA	1672	A	C2-N3-C4	17.37	119.29	110.60
22	BA	1698	A	C2-N3-C4	17.37	119.29	110.60
22	BA	1571	A	N1-C6-N6	-17.37	108.18	118.60
1	AA	1176	A	N1-C6-N6	-17.37	108.18	118.60
1	AA	1105	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	1654	A	C2-N3-C4	17.36	119.28	110.60
1	AA	520	A	C2-N3-C4	17.36	119.28	110.60
22	BA	2117	A	N1-C6-N6	-17.36	108.18	118.60
22	BA	2781	A	N1-C6-N6	-17.36	108.19	118.60
1	AA	1150	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	789	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	95	A	N1-C2-N3	-17.35	120.62	129.30
22	BA	1046	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	739	A	N1-C6-N6	-17.35	108.19	118.60
1	AA	539	A	N1-C6-N6	-17.34	108.19	118.60
22	BA	627	A	N1-C6-N6	-17.34	108.19	118.60
22	BA	1089	A	N1-C6-N6	-17.34	108.20	118.60
22	BA	668	A	C2-N3-C4	17.34	119.27	110.60
22	BA	2560	A	N1-C6-N6	-17.34	108.20	118.60
23	BB	45	A	N1-C2-N3	-17.34	120.63	129.30
1	AA	573	A	C2-N3-C4	17.34	119.27	110.60
1	AA	452	A	N1-C6-N6	-17.33	108.20	118.60
22	BA	685	A	N1-C2-N3	-17.33	120.63	129.30
22	BA	1275	A	C2-N3-C4	17.33	119.27	110.60
1	AA	192	A	N1-C2-N3	-17.33	120.63	129.30
22	BA	2377	A	N1-C2-N3	-17.33	120.64	129.30
22	BA	2725	A	N1-C6-N6	-17.33	108.20	118.60
22	BA	2366	A	C2-N3-C4	17.33	119.26	110.60
1	AA	1480	A	C2-N3-C4	17.32	119.26	110.60
22	BA	743	A	N1-C6-N6	-17.32	108.21	118.60
1	AA	51	A	C2-N3-C4	17.32	119.26	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	246	A	C2-N3-C4	17.32	119.26	110.60
22	BA	1504	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	1086	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	2868	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	2037	A	C2-N3-C4	17.31	119.25	110.60
1	AA	179	A	C2-N3-C4	17.31	119.25	110.60
22	BA	104	A	N1-C6-N6	-17.31	108.22	118.60
22	BA	603	A	C2-N3-C4	17.31	119.25	110.60
22	BA	1080	A	N1-C2-N3	-17.30	120.65	129.30
1	AA	338	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	278	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	1679	A	C2-N3-C4	17.30	119.25	110.60
22	BA	1801	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	2247	A	N1-C6-N6	-17.30	108.22	118.60
1	AA	873	A	N1-C6-N6	-17.29	108.22	118.60
1	AA	1229	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	1580	A	C2-N3-C4	17.29	119.24	110.60
1	AA	572	A	C2-N3-C4	17.28	119.24	110.60
22	BA	996	A	C2-N3-C4	17.28	119.24	110.60
22	BA	2654	A	N1-C6-N6	-17.28	108.23	118.60
23	BB	29	A	N1-C2-N3	-17.28	120.66	129.30
1	AA	199	A	N1-C6-N6	-17.28	108.23	118.60
22	BA	279	A	C2-N3-C4	17.28	119.24	110.60
22	BA	1872	A	N1-C2-N3	-17.28	120.66	129.30
1	AA	1329	A	C2-N3-C4	17.27	119.24	110.60
22	BA	1739	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	144	A	C2-N3-C4	17.27	119.23	110.60
23	BB	115	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	1503	A	N1-C6-N6	-17.26	108.24	118.60
1	AA	655	A	N1-C2-N3	-17.26	120.67	129.30
22	BA	2614	A	N1-C6-N6	-17.26	108.24	118.60
23	BB	34	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	844	A	C2-N3-C4	17.25	119.23	110.60
22	BA	1866	A	C2-N3-C4	17.25	119.22	110.60
1	AA	1250	A	N1-C6-N6	-17.25	108.25	118.60
1	AA	1256	A	N1-C6-N6	-17.24	108.26	118.60
22	BA	575	A	N1-C6-N6	-17.23	108.26	118.60
1	AA	1044	A	N1-C6-N6	-17.23	108.26	118.60
22	BA	2469	A	N1-C6-N6	-17.23	108.26	118.60
1	AA	747	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	2020	A	N1-C6-N6	-17.22	108.27	118.60
1	AA	19	A	N1-C6-N6	-17.22	108.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	143	A	C2-N3-C4	17.21	119.21	110.60
1	AA	1441	A	N1-C6-N6	-17.21	108.28	118.60
1	AA	1287	A	C2-N3-C4	17.20	119.20	110.60
22	BA	415	A	N1-C2-N3	-17.20	120.70	129.30
1	AA	1117	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	362	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	1069	A	N1-C2-N3	-17.19	120.70	129.30
22	BA	2288	A	N1-C6-N6	-17.19	108.28	118.60
1	AA	19	A	N1-C2-N3	-17.19	120.70	129.30
22	BA	1307	A	N1-C6-N6	-17.18	108.29	118.60
22	BA	1373	A	N1-C6-N6	-17.18	108.29	118.60
1	AA	1117	A	C2-N3-C4	17.18	119.19	110.60
22	BA	829	A	N1-C6-N6	-17.18	108.30	118.60
1	AA	1360	A	N1-C2-N3	-17.17	120.71	129.30
1	AA	1252	A	N1-C6-N6	-17.17	108.30	118.60
22	BA	1848	A	C2-N3-C4	17.17	119.18	110.60
22	BA	1502	A	N1-C6-N6	-17.16	108.30	118.60
22	BA	2468	A	N1-C6-N6	-17.16	108.30	118.60
22	BA	1885	A	N1-C6-N6	-17.16	108.30	118.60
22	BA	2497	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	2654	A	C2-N3-C4	17.16	119.18	110.60
22	BA	2820	A	N1-C6-N6	-17.16	108.30	118.60
22	BA	2679	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	28	A	C2-N3-C4	17.16	119.18	110.60
22	BA	1593	A	N1-C6-N6	-17.15	108.31	118.60
22	BA	2634	A	N1-C6-N6	-17.15	108.31	118.60
22	BA	819	A	N1-C6-N6	-17.14	108.32	118.60
22	BA	1739	A	N1-C6-N6	-17.14	108.32	118.60
22	BA	348	A	C2-N3-C4	17.13	119.17	110.60
22	BA	586	A	C2-N3-C4	17.13	119.17	110.60
55	B8	69	A	N1-C6-N6	-17.13	108.32	118.60
1	AA	1349	A	N1-C6-N6	-17.12	108.33	118.60
1	AA	66	A	N1-C2-N3	-17.12	120.74	129.30
1	AA	1163	A	N1-C2-N3	-17.11	120.74	129.30
22	BA	1029	A	C2-N3-C4	17.11	119.16	110.60
22	BA	1759	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	2705	A	C2-N3-C4	17.11	119.16	110.60
22	BA	1808	A	N1-C6-N6	-17.10	108.34	118.60
22	BA	2741	A	C2-N3-C4	17.10	119.15	110.60
22	BA	1057	A	C2-N3-C4	17.10	119.15	110.60
22	BA	5	A	N1-C6-N6	-17.10	108.34	118.60
22	BA	1616	A	N1-C6-N6	-17.10	108.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1784	A	N1-C6-N6	-17.09	108.34	118.60
22	BA	2051	A	N1-C6-N6	-17.09	108.35	118.60
22	BA	1871	A	N1-C6-N6	-17.08	108.35	118.60
1	AA	1256	A	C2-N3-C4	17.08	119.14	110.60
22	BA	404	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	167	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	911	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	1175	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	63	A	N1-C6-N6	-17.07	108.36	118.60
1	AA	59	A	N1-C6-N6	-17.06	108.36	118.60
22	BA	2662	A	N1-C6-N6	-17.06	108.36	118.60
22	BA	471	A	N1-C6-N6	-17.06	108.36	118.60
22	BA	1821	A	C2-N3-C4	17.05	119.13	110.60
22	BA	541	A	N1-C2-N3	-17.05	120.78	129.30
22	BA	1327	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	2268	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	1936	A	N1-C6-N6	-17.04	108.38	118.60
1	AA	1046	A	N1-C2-N3	-17.03	120.79	129.30
22	BA	2392	A	C2-N3-C4	17.02	119.11	110.60
1	AA	1055	A	N1-C6-N6	-17.02	108.39	118.60
1	AA	1227	A	C2-N3-C4	17.02	119.11	110.60
22	BA	1548	A	N1-C6-N6	-17.02	108.39	118.60
1	AA	10	A	N1-C6-N6	-17.02	108.39	118.60
22	BA	1010	A	N1-C6-N6	-17.02	108.39	118.60
22	BA	1469	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	910	A	N1-C6-N6	-17.01	108.39	118.60
1	AA	190	A	N1-C2-N3	-17.01	120.80	129.30
1	AA	300	A	C2-N3-C4	17.01	119.10	110.60
22	BA	2005	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	507	A	N1-C6-N6	-17.01	108.40	118.60
1	AA	994	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	197	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	522	A	N1-C6-N6	-17.00	108.40	118.60
1	AA	228	A	N1-C6-N6	-16.99	108.41	118.60
23	BB	104	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	1010	A	C2-N3-C4	16.98	119.09	110.60
22	BA	1028	A	N1-C6-N6	-16.98	108.41	118.60
23	BB	119	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	2322	A	C2-N3-C4	16.97	119.09	110.60
22	BA	144	A	N1-C2-N3	-16.97	120.81	129.30
22	BA	1434	A	C2-N3-C4	16.97	119.09	110.60
22	BA	1722	A	C2-N3-C4	16.97	119.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1256	A	N1-C2-N3	-16.97	120.82	129.30
22	BA	1272	A	C2-N3-C4	16.97	119.08	110.60
22	BA	2284	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	829	A	C2-N3-C4	16.96	119.08	110.60
1	AA	120	A	N1-C6-N6	-16.96	108.43	118.60
22	BA	42	A	N1-C6-N6	-16.95	108.43	118.60
22	BA	501	A	N1-C6-N6	-16.95	108.43	118.60
22	BA	505	A	N1-C6-N6	-16.94	108.43	118.60
22	BA	1040	A	N1-C6-N6	-16.94	108.44	118.60
22	BA	233	A	C2-N3-C4	16.94	119.07	110.60
1	AA	938	A	N1-C2-N3	-16.94	120.83	129.30
1	AA	608	A	N1-C6-N6	-16.94	108.44	118.60
22	BA	2614	A	N1-C2-N3	-16.93	120.83	129.30
1	AA	1311	A	N1-C6-N6	-16.93	108.44	118.60
22	BA	793	A	N1-C6-N6	-16.93	108.44	118.60
1	AA	1080	A	N1-C6-N6	-16.92	108.45	118.60
22	BA	1810	A	N1-C2-N3	-16.92	120.84	129.30
1	AA	349	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	270	A	N1-C6-N6	-16.91	108.45	118.60
22	BA	472	A	C2-N3-C4	16.91	119.05	110.60
22	BA	91	A	C2-N3-C4	16.91	119.05	110.60
22	BA	608	A	N1-C6-N6	-16.90	108.46	118.60
22	BA	2900	A	C2-N3-C4	16.90	119.05	110.60
1	AA	1081	A	N1-C6-N6	-16.90	108.46	118.60
22	BA	278	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	2497	A	N1-C6-N6	-16.90	108.46	118.60
22	BA	1431	A	N1-C6-N6	-16.89	108.47	118.60
1	AA	262	A	N1-C6-N6	-16.88	108.47	118.60
22	BA	981	A	N1-C6-N6	-16.88	108.47	118.60
22	BA	1977	A	C2-N3-C4	16.88	119.04	110.60
1	AA	383	A	N1-C2-N3	-16.87	120.86	129.30
22	BA	705	A	N1-C6-N6	-16.87	108.48	118.60
1	AA	718	A	N1-C6-N6	-16.87	108.48	118.60
1	AA	1499	A	N1-C6-N6	-16.87	108.48	118.60
1	AA	383	A	C2-N3-C4	16.86	119.03	110.60
22	BA	2700	A	N1-C2-N3	-16.86	120.87	129.30
23	BB	29	A	N1-C6-N6	-16.86	108.48	118.60
22	BA	1301	A	N1-C6-N6	-16.86	108.49	118.60
1	AA	1332	A	N1-C2-N3	-16.85	120.87	129.30
1	AA	1146	A	N1-C6-N6	-16.85	108.49	118.60
1	AA	366	A	N1-C6-N6	-16.84	108.49	118.60
22	BA	1496	A	N1-C6-N6	-16.84	108.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	872	A	N1-C6-N6	-16.84	108.50	118.60
1	AA	1396	A	N1-C6-N6	-16.84	108.50	118.60
22	BA	282	A	N1-C2-N3	-16.84	120.88	129.30
55	B8	76	A	N1-C2-N3	-16.83	120.88	129.30
1	AA	696	A	N1-C6-N6	-16.83	108.50	118.60
22	BA	1848	A	N1-C2-N3	-16.83	120.89	129.30
22	BA	1808	A	C2-N3-C4	16.83	119.01	110.60
1	AA	975	A	N1-C6-N6	-16.83	108.50	118.60
1	AA	459	A	N1-C6-N6	-16.82	108.50	118.60
1	AA	1171	A	N1-C2-N3	-16.82	120.89	129.30
1	AA	1188	A	N1-C6-N6	-16.82	108.51	118.60
1	AA	523	A	N1-C6-N6	-16.82	108.51	118.60
22	BA	197	A	C2-N3-C4	16.82	119.01	110.60
1	AA	199	A	N1-C2-N3	-16.81	120.89	129.30
22	BA	101	A	N1-C6-N6	-16.81	108.51	118.60
22	BA	1981	A	C2-N3-C4	16.81	119.00	110.60
1	AA	1418	A	N1-C2-N3	-16.80	120.90	129.30
1	AA	1534	A	N1-C6-N6	-16.80	108.52	118.60
22	BA	1532	A	N1-C6-N6	-16.80	108.52	118.60
1	AA	487	A	N1-C6-N6	-16.80	108.52	118.60
1	AA	1191	A	N1-C6-N6	-16.79	108.53	118.60
22	BA	1000	A	N1-C6-N6	-16.79	108.52	118.60
22	BA	742	A	N1-C6-N6	-16.79	108.53	118.60
22	BA	2598	A	C2-N3-C4	16.78	118.99	110.60
1	AA	1324	A	N1-C6-N6	-16.77	108.54	118.60
22	BA	1143	A	N1-C6-N6	-16.77	108.54	118.60
22	BA	941	A	N1-C6-N6	-16.77	108.54	118.60
22	BA	282	A	C2-N3-C4	16.77	118.98	110.60
22	BA	127	A	N1-C6-N6	-16.76	108.54	118.60
22	BA	2377	A	N1-C6-N6	-16.75	108.55	118.60
1	AA	908	A	N1-C6-N6	-16.75	108.55	118.60
22	BA	1757	A	N1-C6-N6	-16.75	108.55	118.60
1	AA	174	A	N1-C2-N3	-16.74	120.93	129.30
22	BA	1877	A	N1-C6-N6	-16.73	108.56	118.60
22	BA	1073	A	N1-C6-N6	-16.73	108.56	118.60
22	BA	2450	A	N1-C6-N6	-16.73	108.56	118.60
22	BA	2471	A	N1-C2-N3	-16.73	120.94	129.30
1	AA	573	A	N1-C6-N6	-16.72	108.57	118.60
22	BA	632	A	N1-C6-N6	-16.72	108.57	118.60
22	BA	715	A	N1-C6-N6	-16.72	108.57	118.60
23	BB	34	A	N1-C2-N3	-16.72	120.94	129.30
1	AA	746	A	N1-C6-N6	-16.71	108.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	722	A	N1-C6-N6	-16.71	108.57	118.60
1	AA	1513	A	N1-C6-N6	-16.70	108.58	118.60
22	BA	2176	A	N1-C2-N3	-16.70	120.95	129.30
22	BA	2108	A	N1-C2-N3	-16.70	120.95	129.30
1	AA	498	A	N1-C6-N6	-16.69	108.58	118.60
1	AA	167	A	N1-C6-N6	-16.69	108.58	118.60
1	AA	878	A	N1-C6-N6	-16.69	108.59	118.60
22	BA	1275	A	N1-C6-N6	-16.69	108.59	118.60
22	BA	415	A	N1-C6-N6	-16.69	108.59	118.60
22	BA	2392	A	N1-C2-N3	-16.69	120.96	129.30
1	AA	288	A	C2-N3-C4	16.68	118.94	110.60
22	BA	2037	A	N1-C6-N6	-16.68	108.59	118.60
1	AA	794	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	1029	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	1347	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	1664	A	N1-C6-N6	-16.67	108.60	118.60
22	BA	804	A	N1-C6-N6	-16.66	108.61	118.60
1	AA	161	A	N1-C6-N6	-16.65	108.61	118.60
22	BA	507	A	C2-N3-C4	16.64	118.92	110.60
1	AA	983	A	N1-C6-N6	-16.64	108.62	118.60
22	BA	751	A	N1-C6-N6	-16.64	108.62	118.60
22	BA	1809	A	N1-C6-N6	-16.63	108.62	118.60
22	BA	2142	A	N1-C6-N6	-16.63	108.62	118.60
1	AA	694	A	N1-C6-N6	-16.62	108.63	118.60
1	AA	706	A	N1-C2-N3	-16.62	120.99	129.30
22	BA	1241	A	N1-C6-N6	-16.62	108.62	118.60
23	BB	57	A	N1-C6-N6	-16.62	108.63	118.60
1	AA	1170	A	N1-C6-N6	-16.62	108.63	118.60
1	AA	1507	A	N1-C6-N6	-16.61	108.63	118.60
22	BA	483	A	N1-C6-N6	-16.61	108.64	118.60
22	BA	466	A	N1-C6-N6	-16.60	108.64	118.60
1	AA	715	A	N1-C6-N6	-16.59	108.64	118.60
1	AA	743	A	N1-C6-N6	-16.59	108.65	118.60
22	BA	730	A	N1-C6-N6	-16.59	108.65	118.60
22	BA	1246	A	N1-C6-N6	-16.59	108.65	118.60
22	BA	477	A	N1-C6-N6	-16.59	108.65	118.60
22	BA	1866	A	N1-C6-N6	-16.58	108.65	118.60
1	AA	456	A	N1-C6-N6	-16.58	108.65	118.60
22	BA	255	A	N1-C6-N6	-16.57	108.66	118.60
22	BA	833	A	N1-C6-N6	-16.57	108.66	118.60
1	AA	238	A	N1-C2-N3	-16.56	121.02	129.30
1	AA	72	A	N1-C6-N6	-16.55	108.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1418	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	482	A	N1-C2-N3	-16.55	121.03	129.30
22	BA	727	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	1434	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	800	A	C2-N3-C4	16.54	118.87	110.60
22	BA	782	A	C2-N3-C4	16.54	118.87	110.60
22	BA	1569	A	N1-C6-N6	-16.53	108.68	118.60
22	BA	2727	A	N1-C6-N6	-16.53	108.68	118.60
22	BA	131	A	N1-C6-N6	-16.52	108.69	118.60
1	AA	907	A	N1-C6-N6	-16.52	108.69	118.60
22	BA	975	A	N1-C6-N6	-16.51	108.70	118.60
22	BA	2298	A	N1-C6-N6	-16.51	108.69	118.60
22	BA	2154	A	N1-C2-N3	-16.50	121.05	129.30
1	AA	1105	A	N1-C6-N6	-16.50	108.70	118.60
1	AA	32	A	N1-C6-N6	-16.50	108.70	118.60
22	BA	1490	A	N1-C6-N6	-16.49	108.70	118.60
1	AA	356	A	N1-C6-N6	-16.49	108.71	118.60
22	BA	1580	A	N1-C6-N6	-16.49	108.71	118.60
1	AA	923	A	N1-C6-N6	-16.48	108.71	118.60
22	BA	2471	A	N1-C6-N6	-16.48	108.71	118.60
1	AA	1418	A	C2-N3-C4	16.47	118.84	110.60
22	BA	422	A	N1-C6-N6	-16.47	108.72	118.60
22	BA	2082	A	N1-C6-N6	-16.46	108.72	118.60
1	AA	546	A	N1-C6-N6	-16.46	108.72	118.60
22	BA	1552	A	N1-C6-N6	-16.46	108.73	118.60
1	AA	790	A	N1-C6-N6	-16.45	108.73	118.60
22	BA	2757	A	N1-C6-N6	-16.45	108.73	118.60
22	BA	368	A	N1-C6-N6	-16.43	108.74	118.60
22	BA	2733	A	N1-C6-N6	-16.42	108.75	118.60
22	BA	2386	A	C2-N3-C4	16.41	118.81	110.60
22	BA	782	A	N1-C2-N3	-16.41	121.10	129.30
1	AA	1299	A	N1-C6-N6	-16.39	108.77	118.60
22	BA	2378	A	N1-C6-N6	-16.38	108.77	118.60
22	BA	2077	A	N1-C6-N6	-16.36	108.78	118.60
1	AA	1502	A	C2-N3-C4	16.36	118.78	110.60
22	BA	176	A	N1-C6-N6	-16.36	108.79	118.60
1	AA	279	A	N1-C6-N6	-16.35	108.79	118.60
1	AA	460	A	N1-C6-N6	-16.34	108.79	118.60
1	AA	98	A	N1-C2-N3	-16.34	121.13	129.30
1	AA	1152	A	N1-C6-N6	-16.32	108.81	118.60
22	BA	19	A	N1-C2-N3	-16.31	121.14	129.30
22	BA	52	A	N1-C6-N6	-16.31	108.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1603	A	N1-C6-N6	-16.31	108.81	118.60
1	AA	1169	A	N1-C6-N6	-16.31	108.81	118.60
1	AA	300	A	N1-C2-N3	-16.30	121.15	129.30
22	BA	1847	A	N1-C6-N6	-16.30	108.82	118.60
22	BA	1596	A	N1-C6-N6	-16.29	108.83	118.60
22	BA	173	A	N1-C6-N6	-16.27	108.83	118.60
22	BA	1969	A	C2-N3-C4	16.27	118.74	110.60
22	BA	1608	A	N1-C6-N6	-16.26	108.84	118.60
1	AA	279	A	C2-N3-C4	16.26	118.73	110.60
22	BA	2019	A	C2-N3-C4	16.26	118.73	110.60
1	AA	535	A	N1-C6-N6	-16.26	108.85	118.60
22	BA	654	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	1027	A	C2-N3-C4	16.25	118.73	110.60
22	BA	633	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	1672	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	2366	A	N1-C6-N6	-16.23	108.86	118.60
1	AA	468	A	N1-C6-N6	-16.23	108.86	118.60
22	BA	2268	A	C2-N3-C4	16.22	118.71	110.60
1	AA	1163	A	N1-C6-N6	-16.20	108.88	118.60
22	BA	626	A	N1-C6-N6	-16.20	108.88	118.60
22	BA	1676	A	C2-N3-C4	16.20	118.70	110.60
1	AA	498	A	N1-C2-N3	-16.20	121.20	129.30
22	BA	959	A	N1-C6-N6	-16.20	108.88	118.60
22	BA	1246	A	N1-C2-N3	-16.18	121.21	129.30
1	AA	579	A	N1-C6-N6	-16.18	108.89	118.60
22	BA	1336	A	N1-C6-N6	-16.18	108.89	118.60
1	AA	1019	A	N1-C6-N6	-16.17	108.90	118.60
22	BA	227	A	N1-C6-N6	-16.17	108.90	118.60
22	BA	279	A	N1-C6-N6	-16.17	108.90	118.60
22	BA	2042	A	N1-C6-N6	-16.16	108.90	118.60
22	BA	2900	A	N1-C6-N6	-16.15	108.91	118.60
22	BA	1901	A	N1-C6-N6	-16.15	108.91	118.60
22	BA	2821	A	N1-C6-N6	-16.14	108.92	118.60
22	BA	127	A	C2-N3-C4	16.13	118.67	110.60
22	BA	155	A	N1-C6-N6	-16.13	108.92	118.60
22	BA	2792	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	1508	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	980	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	920	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	1754	A	N1-C6-N6	-16.11	108.93	118.60
1	AA	1102	A	N1-C6-N6	-16.11	108.94	118.60
22	BA	1722	A	N1-C6-N6	-16.11	108.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2097	A	N1-C6-N6	-16.10	108.94	118.60
22	BA	1365	A	N1-C6-N6	-16.10	108.94	118.60
22	BA	52	A	C2-N3-C4	16.10	118.65	110.60
22	BA	470	A	N1-C6-N6	-16.08	108.95	118.60
22	BA	1384	A	N1-C6-N6	-16.08	108.95	118.60
22	BA	1302	A	N1-C6-N6	-16.07	108.96	118.60
22	BA	1302	A	C2-N3-C4	16.06	118.63	110.60
22	BA	91	A	N1-C6-N6	-16.06	108.96	118.60
1	AA	906	A	N1-C6-N6	-16.04	108.98	118.60
22	BA	734	A	N1-C6-N6	-16.04	108.98	118.60
22	BA	689	A	N1-C6-N6	-16.03	108.98	118.60
22	BA	2095	A	N1-C6-N6	-16.03	108.98	118.60
22	BA	2565	A	N1-C6-N6	-16.03	108.98	118.60
1	AA	1197	A	N1-C6-N6	-16.02	108.99	118.60
23	BB	66	A	N1-C2-N3	-16.02	121.29	129.30
22	BA	2183	A	N1-C6-N6	-16.01	108.99	118.60
1	AA	101	A	N1-C2-N3	-16.01	121.30	129.30
22	BA	2879	A	N1-C6-N6	-16.01	109.00	118.60
1	AA	964	A	N1-C6-N6	-16.00	109.00	118.60
1	AA	371	A	N1-C6-N6	-16.00	109.00	118.60
22	BA	1470	A	N1-C6-N6	-16.00	109.00	118.60
22	BA	2273	A	N1-C6-N6	-15.99	109.00	118.60
22	BA	2682	A	N1-C6-N6	-15.98	109.01	118.60
22	BA	191	A	N1-C6-N6	-15.98	109.01	118.60
1	AA	1332	A	C2-N3-C4	15.97	118.58	110.60
22	BA	1899	A	C2-N3-C4	15.97	118.58	110.60
1	AA	1021	A	N1-C2-N3	-15.96	121.32	129.30
22	BA	1528	A	N1-C6-N6	-15.96	109.02	118.60
1	AA	411	A	N1-C6-N6	-15.96	109.03	118.60
23	BB	73	A	N1-C6-N6	-15.96	109.03	118.60
22	BA	384	A	N1-C6-N6	-15.94	109.03	118.60
22	BA	2721	A	N1-C6-N6	-15.95	109.03	118.60
1	AA	353	A	N1-C6-N6	-15.94	109.04	118.60
22	BA	2432	A	C2-N3-C4	15.93	118.57	110.60
1	AA	80	A	N1-C6-N6	-15.93	109.04	118.60
1	AA	1261	A	N1-C6-N6	-15.93	109.04	118.60
22	BA	1156	A	N1-C6-N6	-15.93	109.04	118.60
1	AA	923	A	N1-C2-N3	-15.92	121.34	129.30
22	BA	1614	A	C2-N3-C4	15.92	118.56	110.60
22	BA	2602	A	C2-N3-C4	15.92	118.56	110.60
1	AA	746	A	N1-C2-N3	-15.92	121.34	129.30
22	BA	2670	A	N1-C6-N6	-15.91	109.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2176	A	N1-C6-N6	-15.91	109.05	118.60
1	AA	1046	A	N1-C6-N6	-15.91	109.05	118.60
22	BA	2340	A	N1-C6-N6	-15.91	109.06	118.60
22	BA	256	A	N1-C6-N6	-15.89	109.06	118.60
22	BA	943	A	N1-C6-N6	-15.89	109.07	118.60
22	BA	927	A	N1-C6-N6	-15.88	109.07	118.60
22	BA	2426	A	N1-C6-N6	-15.88	109.07	118.60
22	BA	1009	A	N1-C6-N6	-15.87	109.08	118.60
1	AA	329	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	2054	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	1090	A	N1-C6-N6	-15.84	109.09	118.60
22	BA	513	A	N1-C6-N6	-15.83	109.10	118.60
22	BA	505	A	C2-N3-C4	15.82	118.51	110.60
22	BA	1977	A	N1-C6-N6	-15.80	109.12	118.60
22	BA	2184	A	N1-C6-N6	-15.79	109.12	118.60
22	BA	1654	A	N1-C6-N6	-15.77	109.14	118.60
1	AA	609	A	N1-C6-N6	-15.77	109.14	118.60
22	BA	643	A	N1-C6-N6	-15.77	109.14	118.60
22	BA	2886	A	N1-C6-N6	-15.75	109.15	118.60
22	BA	1027	A	N1-C6-N6	-15.74	109.15	118.60
1	AA	430	A	N1-C6-N6	-15.73	109.16	118.60
1	AA	1236	A	N1-C6-N6	-15.73	109.16	118.60
22	BA	1054	A	N1-C6-N6	-15.72	109.17	118.60
22	BA	2900	A	N1-C2-N3	-15.69	121.45	129.30
22	BA	1872	A	N1-C6-N6	-15.66	109.20	118.60
1	AA	190	A	N1-C6-N6	-15.64	109.22	118.60
1	AA	1508	A	N1-C6-N6	-15.63	109.22	118.60
22	BA	1676	A	N1-C6-N6	-15.63	109.22	118.60
22	BA	2433	A	N1-C6-N6	-15.62	109.23	118.60
1	AA	1483	A	N1-C6-N6	-15.61	109.23	118.60
22	BA	282	A	N1-C6-N6	-15.61	109.24	118.60
1	AA	441	A	N1-C6-N6	-15.60	109.24	118.60
22	BA	972	A	N1-C6-N6	-15.59	109.25	118.60
22	BA	1189	A	N1-C6-N6	-15.58	109.25	118.60
22	BA	1287	A	N1-C6-N6	-15.57	109.26	118.60
22	BA	2598	A	N1-C6-N6	-15.56	109.27	118.60
22	BA	255	A	C2-N3-C4	15.52	118.36	110.60
22	BA	2101	A	N1-C2-N3	-15.51	121.54	129.30
22	BA	1938	A	N1-C6-N6	-15.49	109.30	118.60
22	BA	404	A	C2-N3-C4	15.46	118.33	110.60
1	AA	66	A	N1-C6-N6	-15.45	109.33	118.60
22	BA	1848	A	N1-C6-N6	-15.45	109.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	996	A	N1-C6-N6	-15.44	109.34	118.60
1	AA	1332	A	N1-C6-N6	-15.44	109.34	118.60
22	BA	2459	A	N1-C6-N6	-15.41	109.35	118.60
22	BA	2108	A	N1-C6-N6	-15.38	109.37	118.60
22	BA	1264	A	N1-C6-N6	-15.36	109.38	118.60
1	AA	1507	A	N1-C2-N3	-15.33	121.63	129.30
22	BA	1626	A	N1-C6-N6	-15.33	109.40	118.60
22	BA	2602	A	N1-C2-N3	-15.30	121.65	129.30
22	BA	2407	A	N1-C6-N6	-15.29	109.43	118.60
22	BA	2587	A	N1-C6-N6	-15.26	109.45	118.60
22	BA	1144	A	N1-C6-N6	-15.25	109.45	118.60
23	BB	109	A	N1-C6-N6	-15.25	109.45	118.60
1	AA	767	A	N1-C6-N6	-15.24	109.46	118.60
1	AA	814	A	N1-C6-N6	-15.23	109.46	118.60
1	AA	1201	A	N1-C2-N3	-15.21	121.70	129.30
22	BA	1773	A	N1-C6-N6	-15.19	109.48	118.60
22	BA	391	A	N1-C6-N6	-15.19	109.49	118.60
22	BA	1854	A	N1-C6-N6	-15.15	109.51	118.60
22	BA	1745	A	N1-C6-N6	-15.15	109.51	118.60
1	AA	533	A	N1-C2-N3	-15.14	121.73	129.30
22	BA	1969	A	N1-C6-N6	-15.10	109.54	118.60
22	BA	251	A	N1-C6-N6	-15.07	109.56	118.60
23	BB	59	A	N1-C6-N6	-15.05	109.57	118.60
23	BB	66	A	N1-C6-N6	-15.00	109.60	118.60
22	BA	2059	A	N1-C6-N6	-14.94	109.64	118.60
1	AA	162	A	N1-C6-N6	-14.92	109.65	118.60
1	AA	1219	A	N1-C6-N6	-14.91	109.66	118.60
22	BA	1678	A	N1-C6-N6	-14.91	109.66	118.60
22	BA	1987	A	N7-C8-N9	-14.91	106.35	113.80
1	AA	1468	A	N1-C6-N6	-14.89	109.66	118.60
22	BA	1572	A	N1-C6-N6	-14.89	109.67	118.60
1	AA	119	A	N7-C8-N9	-14.88	106.36	113.80
22	BA	401	A	N1-C6-N6	-14.84	109.70	118.60
22	BA	2799	A	N1-C6-N6	-14.78	109.73	118.60
22	BA	2287	A	N1-C6-N6	-14.77	109.74	118.60
22	BA	1086	A	N1-C2-N3	-14.77	121.92	129.30
22	BA	677	A	N1-C6-N6	-14.75	109.75	118.60
22	BA	453	A	N1-C6-N6	-14.71	109.77	118.60
1	AA	98	A	N1-C6-N6	-14.66	109.81	118.60
22	BA	482	A	C2-N3-C4	14.58	117.89	110.60
22	BA	1787	A	N1-C6-N6	-14.53	109.88	118.60
22	BA	820	A	N1-C6-N6	-14.51	109.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2899	A	N1-C6-N6	-14.47	109.92	118.60
22	BA	1213	A	N1-C6-N6	-14.45	109.93	118.60
22	BA	1783	A	N7-C8-N9	-14.42	106.59	113.80
22	BA	675	A	N1-C6-N6	-14.41	109.95	118.60
22	BA	1668	A	C5-C6-N6	14.40	135.22	123.70
1	AA	130	A	N1-C6-N6	-14.38	109.97	118.60
1	AA	1201	A	N1-C6-N6	-14.37	109.98	118.60
1	AA	101	A	C5-C6-N6	14.36	135.19	123.70
1	AA	759	A	N7-C8-N9	-14.35	106.62	113.80
22	BA	479	A	N7-C8-N9	-14.30	106.65	113.80
22	BA	2829	A	N7-C8-N9	-14.25	106.67	113.80
22	BA	213	A	N7-C8-N9	-14.23	106.68	113.80
23	BB	101	A	N3-C4-C5	-14.22	116.84	126.80
1	AA	116	A	N1-C6-N6	-14.22	110.07	118.60
22	BA	1027	A	N7-C8-N9	-14.21	106.69	113.80
22	BA	2435	A	N7-C8-N9	-14.21	106.70	113.80
22	BA	2632	A	N7-C8-N9	-14.06	106.77	113.80
22	BA	749	A	N7-C8-N9	-14.06	106.77	113.80
22	BA	2432	A	N1-C6-N6	-13.98	110.21	118.60
22	BA	1385	A	N7-C8-N9	-13.97	106.82	113.80
1	AA	792	A	N7-C8-N9	-13.95	106.82	113.80
1	AA	300	A	N1-C6-N6	-13.95	110.23	118.60
22	BA	979	A	N7-C8-N9	-13.94	106.83	113.80
1	AA	520	A	C5-C6-N6	13.94	134.85	123.70
23	BB	59	A	N1-C2-N3	-13.90	122.35	129.30
22	BA	2062	A	C5-C6-N6	13.89	134.81	123.70
22	BA	371	A	N7-C8-N9	-13.89	106.85	113.80
22	BA	2665	A	N7-C8-N9	-13.85	106.88	113.80
22	BA	1204	A	C5-C6-N6	13.77	134.72	123.70
23	BB	66	A	C2-N3-C4	13.77	117.49	110.60
22	BA	1614	A	N1-C6-N6	-13.77	110.34	118.60
22	BA	1165	A	N7-C8-N9	-13.77	106.92	113.80
23	BB	99	A	C5-C6-N6	13.77	134.71	123.70
22	BA	1937	A	C5-C6-N6	13.69	134.65	123.70
22	BA	2033	A	C5-C6-N6	13.68	134.64	123.70
22	BA	1420	A	N7-C8-N9	-13.65	106.97	113.80
22	BA	1652	A	N7-C8-N9	-13.65	106.97	113.80
22	BA	689	A	N7-C8-N9	-13.63	106.98	113.80
22	BA	2750	A	N7-C8-N9	-13.62	106.99	113.80
1	AA	583	A	N7-C8-N9	-13.62	106.99	113.80
22	BA	983	A	N1-C6-N6	-13.61	110.43	118.60
22	BA	2823	A	N7-C8-N9	-13.59	107.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1596	A	N7-C8-N9	-13.58	107.01	113.80
1	AA	1213	A	N7-C8-N9	-13.56	107.02	113.80
22	BA	1247	A	N7-C8-N9	-13.56	107.02	113.80
1	AA	69	G	C5'-C4'-O4'	13.54	125.35	109.10
22	BA	2340	A	N7-C8-N9	-13.54	107.03	113.80
22	BA	2883	A	N7-C8-N9	-13.53	107.03	113.80
22	BA	2335	A	N7-C8-N9	-13.51	107.04	113.80
22	BA	222	A	N7-C8-N9	-13.48	107.06	113.80
22	BA	2758	A	N7-C8-N9	-13.48	107.06	113.80
22	BA	668	A	N7-C8-N9	-13.47	107.06	113.80
22	BA	1690	A	C5-C6-N6	13.47	134.48	123.70
1	AA	1503	A	N7-C8-N9	-13.47	107.06	113.80
22	BA	2821	A	N7-C8-N9	-13.47	107.07	113.80
1	AA	1429	A	N7-C8-N9	-13.46	107.07	113.80
1	AA	1499	A	N7-C8-N9	-13.44	107.08	113.80
22	BA	526	A	C5-C6-N6	13.43	134.44	123.70
22	BA	1641	A	C5-C6-N6	13.43	134.44	123.70
22	BA	2388	A	N7-C8-N9	-13.43	107.09	113.80
22	BA	1308	A	N7-C8-N9	-13.42	107.09	113.80
22	BA	2327	A	C5-C6-N6	13.41	134.43	123.70
22	BA	2602	A	C5-C6-N6	13.41	134.43	123.70
22	BA	1866	A	N7-C8-N9	-13.40	107.10	113.80
1	AA	383	A	N1-C6-N6	-13.39	110.57	118.60
22	BA	262	A	N7-C8-N9	-13.38	107.11	113.80
1	AA	1285	A	N7-C8-N9	-13.37	107.11	113.80
23	BB	34	A	N7-C8-N9	-13.37	107.11	113.80
22	BA	1032	A	N7-C8-N9	-13.37	107.12	113.80
1	AA	1502	A	N7-C8-N9	-13.36	107.12	113.80
22	BA	1630	A	C5-C6-N6	13.36	134.39	123.70
22	BA	693	A	N7-C8-N9	-13.35	107.12	113.80
22	BA	528	A	C5-C6-N6	13.35	134.38	123.70
1	AA	468	A	N7-C8-N9	-13.35	107.13	113.80
22	BA	1009	A	N7-C8-N9	-13.35	107.13	113.80
1	AA	802	A	N7-C8-N9	-13.33	107.14	113.80
1	AA	411	A	N7-C8-N9	-13.33	107.14	113.80
1	AA	243	A	C5-C6-N6	13.31	134.35	123.70
22	BA	1805	A	N7-C8-N9	-13.31	107.14	113.80
1	AA	1105	A	N7-C8-N9	-13.30	107.15	113.80
22	BA	1672	A	N7-C8-N9	-13.29	107.16	113.80
22	BA	2482	A	N7-C8-N9	-13.29	107.16	113.80
22	BA	677	A	N7-C8-N9	-13.29	107.16	113.80
55	B8	76	A	C5-C6-N6	13.29	134.33	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1580	A	N7-C8-N9	-13.28	107.16	113.80
22	BA	1359	A	C5-C6-N6	13.26	134.31	123.70
22	BA	699	A	C5-C6-N6	13.26	134.31	123.70
22	BA	1802	A	N1-C6-N6	-13.26	110.64	118.60
22	BA	1504	A	N7-C8-N9	-13.26	107.17	113.80
22	BA	126	A	C5-C6-N6	13.25	134.30	123.70
22	BA	471	A	N7-C8-N9	-13.24	107.18	113.80
22	BA	1378	A	C5-C6-N6	13.24	134.29	123.70
1	AA	572	A	N7-C8-N9	-13.23	107.19	113.80
22	BA	845	A	N7-C8-N9	-13.23	107.19	113.80
22	BA	2518	A	N7-C8-N9	-13.22	107.19	113.80
1	AA	461	A	C5-C6-N6	13.22	134.28	123.70
1	AA	1377	A	N7-C8-N9	-13.20	107.20	113.80
22	BA	614	A	N7-C8-N9	-13.19	107.20	113.80
22	BA	1810	A	N1-C6-N6	-13.19	110.69	118.60
22	BA	2657	A	N7-C8-N9	-13.18	107.21	113.80
1	AA	1016	A	N7-C8-N9	-13.17	107.22	113.80
22	BA	352	A	N7-C8-N9	-13.16	107.22	113.80
22	BA	2600	A	N7-C8-N9	-13.16	107.22	113.80
22	BA	83	A	N7-C8-N9	-13.15	107.22	113.80
22	BA	1144	A	N7-C8-N9	-13.15	107.23	113.80
1	AA	915	A	N7-C8-N9	-13.14	107.23	113.80
1	AA	243	A	N7-C8-N9	-13.14	107.23	113.80
22	BA	1275	A	N7-C8-N9	-13.12	107.24	113.80
1	AA	152	A	C5-C6-N6	13.12	134.20	123.70
1	AA	694	A	N7-C8-N9	-13.12	107.24	113.80
1	AA	1362	A	N7-C8-N9	-13.11	107.25	113.80
22	BA	1147	A	N7-C8-N9	-13.11	107.25	113.80
22	BA	2565	A	N7-C8-N9	-13.11	107.25	113.80
22	BA	631	A	N7-C8-N9	-13.09	107.25	113.80
23	BB	59	A	N3-C4-C5	-13.09	117.64	126.80
22	BA	945	A	C5-C6-N6	13.09	134.17	123.70
22	BA	844	A	N7-C8-N9	-13.09	107.26	113.80
22	BA	1509	A	N7-C8-N9	-13.06	107.27	113.80
22	BA	526	A	N7-C8-N9	-13.04	107.28	113.80
22	BA	2212	A	C5-C6-N6	13.04	134.13	123.70
22	BA	89	A	N7-C8-N9	-13.03	107.29	113.80
22	BA	2211	A	N7-C8-N9	-13.03	107.29	113.80
1	AA	901	A	N1-C6-N6	-13.02	110.79	118.60
22	BA	1700	A	N7-C8-N9	-13.02	107.29	113.80
1	AA	1306	A	N7-C8-N9	-13.01	107.29	113.80
22	BA	2052	A	N7-C8-N9	-13.01	107.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	935	A	N7-C8-N9	-13.00	107.30	113.80
1	AA	1275	A	N7-C8-N9	-13.00	107.30	113.80
1	AA	356	A	N7-C8-N9	-12.99	107.30	113.80
22	BA	1378	A	N7-C8-N9	-12.99	107.31	113.80
1	AA	675	A	N7-C8-N9	-12.98	107.31	113.80
22	BA	1566	A	N7-C8-N9	-12.97	107.31	113.80
22	BA	734	A	N7-C8-N9	-12.97	107.32	113.80
22	BA	244	A	C5-C6-N6	12.97	134.07	123.70
22	BA	1419	A	N7-C8-N9	-12.97	107.32	113.80
1	AA	10	A	N7-C8-N9	-12.96	107.32	113.80
1	AA	143	A	N7-C8-N9	-12.96	107.32	113.80
1	AA	1213	A	C5-C6-N6	12.96	134.07	123.70
22	BA	863	A	N7-C8-N9	-12.96	107.32	113.80
1	AA	1035	A	C5-C6-N6	12.95	134.06	123.70
1	AA	1329	A	N7-C8-N9	-12.95	107.32	113.80
1	AA	781	A	N7-C8-N9	-12.95	107.33	113.80
22	BA	800	A	C5-C6-N6	12.94	134.05	123.70
1	AA	78	A	N7-C8-N9	-12.94	107.33	113.80
22	BA	1755	A	N7-C8-N9	-12.94	107.33	113.80
22	BA	2614	A	N3-C4-C5	-12.93	117.75	126.80
22	BA	1591	A	N7-C8-N9	-12.91	107.34	113.80
1	AA	1101	A	N7-C8-N9	-12.91	107.35	113.80
1	AA	253	A	N7-C8-N9	-12.90	107.35	113.80
1	AA	77	A	N7-C8-N9	-12.90	107.35	113.80
22	BA	804	A	N7-C8-N9	-12.90	107.35	113.80
1	AA	554	A	C5-C6-N6	12.89	134.01	123.70
1	AA	71	A	N7-C8-N9	-12.88	107.36	113.80
22	BA	449	A	N7-C8-N9	-12.88	107.36	113.80
1	AA	579	A	N7-C8-N9	-12.88	107.36	113.80
1	AA	68	G	N3-C4-C5	-12.87	122.16	128.60
22	BA	14	A	C5-C6-N6	12.87	134.00	123.70
1	AA	327	A	N7-C8-N9	-12.87	107.37	113.80
1	AA	99	C	N1-C2-O2	12.85	126.61	118.90
1	AA	371	A	N7-C8-N9	-12.85	107.37	113.80
1	AA	1346	A	N7-C8-N9	-12.85	107.37	113.80
22	BA	1858	A	N7-C8-N9	-12.85	107.38	113.80
22	BA	2080	A	N7-C8-N9	-12.85	107.38	113.80
22	BA	2726	A	N7-C8-N9	-12.84	107.38	113.80
22	BA	1508	A	N7-C8-N9	-12.83	107.38	113.80
22	BA	1194	A	N7-C8-N9	-12.83	107.39	113.80
22	BA	1757	A	N7-C8-N9	-12.83	107.39	113.80
1	AA	495	A	N7-C8-N9	-12.82	107.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	994	A	N7-C8-N9	-12.82	107.39	113.80
22	BA	676	A	N7-C8-N9	-12.82	107.39	113.80
22	BA	2670	A	N7-C8-N9	-12.82	107.39	113.80
22	BA	960	A	C5-C6-N6	12.81	133.95	123.70
22	BA	374	A	C5-C6-N6	12.81	133.95	123.70
1	AA	996	A	N7-C8-N9	-12.81	107.40	113.80
22	BA	933	A	C5-C6-N6	12.80	133.94	123.70
22	BA	1133	A	C5-C6-N6	12.80	133.94	123.70
1	AA	393	A	N7-C8-N9	-12.80	107.40	113.80
1	AA	441	A	N7-C8-N9	-12.79	107.40	113.80
22	BA	515	A	N7-C8-N9	-12.79	107.40	113.80
22	BA	1784	A	N7-C8-N9	-12.79	107.40	113.80
22	BA	608	A	N7-C8-N9	-12.79	107.41	113.80
1	AA	320	A	N7-C8-N9	-12.78	107.41	113.80
22	BA	586	A	C5-C6-N6	12.78	133.92	123.70
1	AA	120	A	N7-C8-N9	-12.77	107.41	113.80
22	BA	2042	A	N7-C8-N9	-12.77	107.42	113.80
22	BA	299	A	C5-C6-N6	12.76	133.91	123.70
22	BA	1046	A	N7-C8-N9	-12.76	107.42	113.80
22	BA	1711	A	N7-C8-N9	-12.76	107.42	113.80
22	BA	866	A	N7-C8-N9	-12.76	107.42	113.80
22	BA	1204	A	N7-C8-N9	-12.76	107.42	113.80
22	BA	2287	A	N7-C8-N9	-12.76	107.42	113.80
22	BA	2589	A	N7-C8-N9	-12.76	107.42	113.80
1	AA	349	A	N7-C8-N9	-12.75	107.42	113.80
1	AA	353	A	N7-C8-N9	-12.75	107.43	113.80
22	BA	2449	U	C5-C6-N1	-12.75	116.33	122.70
22	BA	1515	A	C5-C6-N6	12.74	133.90	123.70
1	AA	309	A	N7-C8-N9	-12.74	107.43	113.80
22	BA	721	A	N7-C8-N9	-12.74	107.43	113.80
1	AA	498	A	N3-C4-C5	-12.73	117.89	126.80
1	AA	563	A	C5-C6-N6	12.73	133.89	123.70
1	AA	182	A	N7-C8-N9	-12.73	107.44	113.80
22	BA	53	A	N7-C8-N9	-12.73	107.44	113.80
1	AA	918	A	N7-C8-N9	-12.72	107.44	113.80
22	BA	1789	A	C5-C6-N6	12.72	133.88	123.70
23	BB	101	A	N1-C2-N3	-12.72	122.94	129.30
1	AA	101	A	N7-C8-N9	-12.71	107.44	113.80
1	AA	1408	A	N7-C8-N9	-12.72	107.44	113.80
1	AA	1081	A	N7-C8-N9	-12.71	107.45	113.80
1	AA	766	A	N7-C8-N9	-12.70	107.45	113.80
1	AA	600	A	N7-C8-N9	-12.70	107.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1749	A	N7-C8-N9	-12.69	107.45	113.80
22	BA	1213	A	N7-C8-N9	-12.69	107.45	113.80
1	AA	572	A	C5-C6-N6	12.69	133.85	123.70
22	BA	538	A	N7-C8-N9	-12.69	107.46	113.80
22	BA	344	A	N7-C8-N9	-12.68	107.46	113.80
22	BA	1655	A	N7-C8-N9	-12.68	107.46	113.80
22	BA	1021	A	N3-C4-C5	-12.67	117.93	126.80
22	BA	2602	A	N7-C8-N9	-12.67	107.46	113.80
1	AA	1413	A	N7-C8-N9	-12.67	107.47	113.80
22	BA	1194	A	C5-C6-N6	12.67	133.83	123.70
1	AA	1179	A	N7-C8-N9	-12.66	107.47	113.80
1	AA	282	A	N7-C8-N9	-12.66	107.47	113.80
22	BA	2430	A	C5-C6-N6	12.65	133.82	123.70
22	BA	432	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	1393	A	C5-C6-N6	12.64	133.81	123.70
1	AA	152	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	167	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	1528	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	2471	A	N7-C8-N9	-12.63	107.48	113.80
1	AA	554	A	N7-C8-N9	-12.63	107.48	113.80
22	BA	2766	A	N7-C8-N9	-12.63	107.48	113.80
22	BA	750	A	N7-C8-N9	-12.63	107.49	113.80
22	BA	1354	A	N7-C8-N9	-12.63	107.49	113.80
1	AA	546	A	N7-C8-N9	-12.63	107.49	113.80
22	BA	1772	A	N7-C8-N9	-12.62	107.49	113.80
1	AA	321	A	N7-C8-N9	-12.62	107.49	113.80
22	BA	2070	A	N7-C8-N9	-12.62	107.49	113.80
22	BA	111	A	C5-C6-N6	12.62	133.79	123.70
22	BA	430	A	N7-C8-N9	-12.62	107.49	113.80
1	AA	1117	A	N7-C8-N9	-12.62	107.49	113.80
22	BA	119	A	C5-C6-N6	12.62	133.79	123.70
1	AA	68	G	C6-C5-N7	-12.61	122.83	130.40
22	BA	764	A	C5-C6-N6	12.61	133.79	123.70
1	AA	974	A	N7-C8-N9	-12.61	107.50	113.80
1	AA	1465	A	N7-C8-N9	-12.60	107.50	113.80
22	BA	1981	A	N7-C8-N9	-12.60	107.50	113.80
1	AA	60	A	C5-C6-N6	12.59	133.78	123.70
1	AA	787	A	N7-C8-N9	-12.59	107.50	113.80
1	AA	1340	A	N7-C8-N9	-12.59	107.50	113.80
22	BA	111	A	N7-C8-N9	-12.59	107.50	113.80
22	BA	457	A	N7-C8-N9	-12.59	107.50	113.80
22	BA	1001	A	C5-C6-N6	12.58	133.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	81	A	C5-C6-N6	12.58	133.76	123.70
22	BA	2119	A	C5-C6-N6	12.58	133.76	123.70
1	AA	520	A	N7-C8-N9	-12.58	107.51	113.80
22	BA	1583	A	N7-C8-N9	-12.58	107.51	113.80
1	AA	860	A	N7-C8-N9	-12.57	107.52	113.80
1	AA	414	A	N7-C8-N9	-12.57	107.52	113.80
22	BA	2776	A	C5-C6-N6	12.56	133.75	123.70
22	BA	1098	A	N7-C8-N9	-12.56	107.52	113.80
1	AA	1167	A	N7-C8-N9	-12.56	107.52	113.80
22	BA	13	A	N3-C4-C5	-12.55	118.01	126.80
1	AA	665	A	N7-C8-N9	-12.55	107.52	113.80
1	AA	1179	A	C5-C6-N6	12.54	133.74	123.70
1	AA	408	A	N7-C8-N9	-12.54	107.53	113.80
22	BA	64	A	N7-C8-N9	-12.53	107.53	113.80
22	BA	983	A	N7-C8-N9	-12.53	107.53	113.80
22	BA	1328	A	C5-C6-N6	12.53	133.72	123.70
22	BA	1669	A	C5-C6-N6	12.53	133.72	123.70
22	BA	602	A	N7-C8-N9	-12.52	107.54	113.80
22	BA	1829	A	N3-C4-C5	-12.52	118.04	126.80
22	BA	2333	A	N7-C8-N9	-12.52	107.54	113.80
1	AA	435	A	N7-C8-N9	-12.51	107.54	113.80
22	BA	2376	A	N7-C8-N9	-12.51	107.54	113.80
22	BA	655	A	N7-C8-N9	-12.51	107.55	113.80
1	AA	539	A	N7-C8-N9	-12.51	107.55	113.80
1	AA	1428	A	C5-C6-N6	12.51	133.71	123.70
23	BB	58	A	C5-C6-N6	12.51	133.71	123.70
23	BB	115	A	N7-C8-N9	-12.51	107.55	113.80
22	BA	282	A	N7-C8-N9	-12.50	107.55	113.80
1	AA	535	A	N7-C8-N9	-12.50	107.55	113.80
22	BA	2435	A	C5-C6-N6	12.50	133.70	123.70
22	BA	2513	A	C5-C6-N6	12.50	133.70	123.70
1	AA	155	A	N7-C8-N9	-12.50	107.55	113.80
22	BA	718	A	N7-C8-N9	-12.50	107.55	113.80
1	AA	1246	A	N7-C8-N9	-12.49	107.55	113.80
22	BA	2468	A	N7-C8-N9	-12.49	107.55	113.80
1	AA	274	A	N7-C8-N9	-12.49	107.56	113.80
22	BA	191	A	N7-C8-N9	-12.49	107.56	113.80
22	BA	1129	A	N7-C8-N9	-12.49	107.56	113.80
22	BA	309	A	N7-C8-N9	-12.48	107.56	113.80
22	BA	900	A	N7-C8-N9	-12.48	107.56	113.80
22	BA	2059	A	N7-C8-N9	-12.48	107.56	113.80
22	BA	1717	A	N7-C8-N9	-12.48	107.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	878	A	N7-C8-N9	-12.47	107.56	113.80
22	BA	826	U	OP1-P-O3'	-12.47	77.76	105.20
1	AA	1004	A	N7-C8-N9	-12.47	107.56	113.80
1	AA	8	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	2823	A	C5-C6-N6	12.46	133.67	123.70
22	BA	466	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	2461	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	265	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	541	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	1039	A	N7-C8-N9	-12.46	107.57	113.80
1	AA	1476	A	N7-C8-N9	-12.46	107.57	113.80
23	BB	99	A	N7-C8-N9	-12.45	107.57	113.80
22	BA	1014	A	N7-C8-N9	-12.45	107.58	113.80
1	AA	130	A	N7-C8-N9	-12.45	107.58	113.80
1	AA	499	A	N7-C8-N9	-12.45	107.58	113.80
22	BA	877	A	N7-C8-N9	-12.45	107.58	113.80
22	BA	1301	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	1244	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	2542	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	5	A	N7-C8-N9	-12.43	107.58	113.80
22	BA	529	A	C5-C6-N6	12.43	133.64	123.70
22	BA	825	A	C5-C6-N6	12.42	133.64	123.70
22	BA	2013	A	N7-C8-N9	-12.42	107.59	113.80
1	AA	1428	A	N7-C8-N9	-12.42	107.59	113.80
22	BA	2358	A	N7-C8-N9	-12.42	107.59	113.80
1	AA	1257	A	N7-C8-N9	-12.41	107.59	113.80
22	BA	2810	A	N7-C8-N9	-12.41	107.59	113.80
1	AA	363	A	N7-C8-N9	-12.41	107.59	113.80
1	AA	825	A	N7-C8-N9	-12.41	107.60	113.80
1	AA	1021	A	N7-C8-N9	-12.41	107.60	113.80
1	AA	1433	A	N7-C8-N9	-12.41	107.60	113.80
22	BA	2682	A	N7-C8-N9	-12.41	107.60	113.80
1	AA	160	A	C5-C6-N6	12.40	133.62	123.70
1	AA	373	A	N7-C8-N9	-12.40	107.60	113.80
22	BA	2381	A	C5-C6-N6	12.40	133.62	123.70
23	BB	119	A	N7-C8-N9	-12.40	107.60	113.80
1	AA	228	A	N7-C8-N9	-12.40	107.60	113.80
1	AA	1102	A	N7-C8-N9	-12.40	107.60	113.80
1	AA	1251	A	C5-C6-N6	12.40	133.62	123.70
22	BA	1626	A	N7-C8-N9	-12.39	107.60	113.80
22	BA	788	A	N7-C8-N9	-12.39	107.60	113.80
22	BA	2126	A	N7-C8-N9	-12.39	107.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2241	A	N7-C8-N9	-12.39	107.61	113.80
22	BA	207	A	N7-C8-N9	-12.38	107.61	113.80
22	BA	722	A	N7-C8-N9	-12.38	107.61	113.80
1	AA	608	A	N7-C8-N9	-12.38	107.61	113.80
22	BA	1085	A	N7-C8-N9	-12.37	107.61	113.80
22	BA	1111	A	N7-C8-N9	-12.37	107.61	113.80
22	BA	1593	A	N7-C8-N9	-12.37	107.61	113.80
1	AA	1333	A	N7-C8-N9	-12.37	107.62	113.80
22	BA	905	A	N7-C8-N9	-12.37	107.62	113.80
22	BA	586	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	2031	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	2411	A	N7-C8-N9	-12.36	107.62	113.80
1	AA	1067	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	320	A	N7-C8-N9	-12.35	107.62	113.80
22	BA	1821	A	N7-C8-N9	-12.35	107.63	113.80
22	BA	1367	A	N7-C8-N9	-12.35	107.63	113.80
1	AA	1398	A	N7-C8-N9	-12.34	107.63	113.80
22	BA	2381	A	N7-C8-N9	-12.34	107.63	113.80
1	AA	167	A	N7-C8-N9	-12.34	107.63	113.80
22	BA	1503	A	N7-C8-N9	-12.34	107.63	113.80
1	AA	510	A	N7-C8-N9	-12.34	107.63	113.80
1	AA	1280	A	N7-C8-N9	-12.33	107.63	113.80
22	BA	311	A	C5-C6-N6	12.33	133.57	123.70
22	BA	2173	A	C5-C6-N6	12.33	133.57	123.70
1	AA	1239	A	N7-C8-N9	-12.33	107.64	113.80
22	BA	2412	A	N7-C8-N9	-12.33	107.64	113.80
22	BA	2800	A	C5-C6-N6	12.33	133.56	123.70
22	BA	176	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	1632	A	N7-C8-N9	-12.32	107.64	113.80
1	AA	753	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	42	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	685	A	N3-C4-C5	-12.32	118.18	126.80
22	BA	756	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	1597	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	1966	A	C5-C6-N6	12.32	133.56	123.70
22	BA	1469	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	1977	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	2077	A	N7-C8-N9	-12.32	107.64	113.80
1	AA	1256	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	2835	A	C5-C6-N6	12.31	133.55	123.70
22	BA	2020	A	N7-C8-N9	-12.31	107.64	113.80
1	AA	1480	A	N7-C8-N9	-12.31	107.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	453	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	984	A	C5-C6-N6	12.31	133.55	123.70
22	BA	2090	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	196	A	C5-C6-N6	12.30	133.54	123.70
22	BA	789	A	N7-C8-N9	-12.30	107.65	113.80
22	BA	1821	A	C5-C6-N6	12.30	133.54	123.70
1	AA	119	A	C5-C6-N6	12.29	133.53	123.70
22	BA	447	A	N7-C8-N9	-12.29	107.65	113.80
1	AA	1036	A	N7-C8-N9	-12.29	107.66	113.80
22	BA	2566	A	C5-C6-N6	12.29	133.53	123.70
1	AA	607	A	C5-C6-N6	12.29	133.53	123.70
22	BA	216	A	C5-C6-N6	12.28	133.53	123.70
22	BA	927	A	N7-C8-N9	-12.28	107.66	113.80
1	AA	236	A	N7-C8-N9	-12.28	107.66	113.80
1	AA	1196	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	529	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	802	A	C5-C6-N6	12.28	133.52	123.70
22	BA	1713	A	C5-C6-N6	12.28	133.52	123.70
1	AA	918	A	C5-C6-N6	12.27	133.52	123.70
22	BA	354	A	N7-C8-N9	-12.27	107.67	113.80
22	BA	272	A	N7-C8-N9	-12.27	107.67	113.80
1	AA	74	A	N7-C8-N9	-12.27	107.67	113.80
22	BA	661	A	N7-C8-N9	-12.27	107.67	113.80
22	BA	2327	A	N7-C8-N9	-12.27	107.67	113.80
22	BA	2882	A	C5-C6-N6	12.27	133.51	123.70
22	BA	348	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	52	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	1634	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	2675	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	644	A	N7-C8-N9	-12.25	107.67	113.80
22	BA	2893	A	N7-C8-N9	-12.25	107.67	113.80
1	AA	1368	A	N7-C8-N9	-12.25	107.68	113.80
22	BA	1762	A	C5-C6-N6	12.25	133.50	123.70
1	AA	431	A	C5-C6-N6	12.24	133.49	123.70
22	BA	666	A	N7-C8-N9	-12.24	107.68	113.80
1	AA	171	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	103	A	N7-C8-N9	-12.24	107.68	113.80
1	AA	246	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	699	A	N7-C8-N9	-12.24	107.68	113.80
1	AA	547	A	C5-C6-N6	12.23	133.49	123.70
1	AA	919	A	N7-C8-N9	-12.23	107.68	113.80
22	BA	1609	A	N7-C8-N9	-12.23	107.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	125	A	N7-C8-N9	-12.23	107.69	113.80
22	BA	1040	A	N7-C8-N9	-12.23	107.68	113.80
22	BA	1354	A	C5-C6-N6	12.23	133.48	123.70
22	BA	2829	A	C5-C6-N6	12.23	133.48	123.70
1	AA	364	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	199	A	N7-C8-N9	-12.22	107.69	113.80
1	AA	777	A	C5-C6-N6	12.22	133.47	123.70
22	BA	1490	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	2740	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	2856	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	2281	A	N7-C8-N9	-12.21	107.69	113.80
22	BA	563	A	N7-C8-N9	-12.21	107.69	113.80
22	BA	294	A	N7-C8-N9	-12.21	107.69	113.80
22	BA	1308	A	C5-C6-N6	12.21	133.47	123.70
22	BA	2270	A	N7-C8-N9	-12.21	107.69	113.80
1	AA	250	A	N7-C8-N9	-12.21	107.70	113.80
1	AA	1180	A	N7-C8-N9	-12.21	107.70	113.80
22	BA	1522	A	N7-C8-N9	-12.20	107.70	113.80
22	BA	1722	A	N7-C8-N9	-12.20	107.70	113.80
1	AA	306	A	N7-C8-N9	-12.20	107.70	113.80
22	BA	637	A	N7-C8-N9	-12.19	107.70	113.80
22	BA	910	A	N7-C8-N9	-12.19	107.70	113.80
22	BA	575	A	N7-C8-N9	-12.19	107.70	113.80
22	BA	1434	A	N7-C8-N9	-12.19	107.70	113.80
22	BA	2273	A	N3-C4-C5	-12.19	118.27	126.80
22	BA	196	A	N7-C8-N9	-12.18	107.71	113.80
22	BA	1254	A	C5-C6-N6	12.18	133.44	123.70
22	BA	2335	A	C5-C6-N6	12.18	133.44	123.70
22	BA	2060	A	N7-C8-N9	-12.18	107.71	113.80
22	BA	2572	A	C5-C6-N6	12.18	133.44	123.70
22	BA	1927	A	C5-C6-N6	12.18	133.44	123.70
22	BA	1937	A	N7-C8-N9	-12.17	107.71	113.80
1	AA	1163	A	N7-C8-N9	-12.17	107.72	113.80
22	BA	492	A	C5-C6-N6	12.17	133.43	123.70
22	BA	899	A	N7-C8-N9	-12.16	107.72	113.80
1	AA	1360	A	N7-C8-N9	-12.16	107.72	113.80
22	BA	1932	A	C5-C6-N6	12.16	133.43	123.70
1	AA	71	A	C5-C6-N6	12.15	133.42	123.70
1	AA	596	A	N7-C8-N9	-12.15	107.72	113.80
22	BA	2753	A	C5-C6-N6	12.15	133.42	123.70
1	AA	687	A	N7-C8-N9	-12.15	107.73	113.80
1	AA	621	A	N7-C8-N9	-12.14	107.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1431	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	514	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	2297	A	C5-C6-N6	12.14	133.42	123.70
22	BA	1652	A	C5-C6-N6	12.14	133.41	123.70
22	BA	1393	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	2227	A	C5-C6-N6	12.14	133.41	123.70
1	AA	1155	A	N7-C8-N9	-12.13	107.73	113.80
22	BA	310	A	N7-C8-N9	-12.13	107.74	113.80
1	AA	197	A	N7-C8-N9	-12.12	107.74	113.80
1	AA	493	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	821	A	C5-C6-N6	12.12	133.40	123.70
22	BA	2531	A	N7-C8-N9	-12.12	107.74	113.80
1	AA	777	A	N7-C8-N9	-12.12	107.74	113.80
1	AA	1016	A	C5-C6-N6	12.12	133.40	123.70
22	BA	2883	A	C5-C6-N6	12.12	133.40	123.70
1	AA	1441	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	457	A	C5-C6-N6	12.12	133.39	123.70
22	BA	2088	A	N7-C8-N9	-12.11	107.74	113.80
22	BA	933	A	N7-C8-N9	-12.11	107.75	113.80
22	BA	1276	A	N7-C8-N9	-12.11	107.74	113.80
22	BA	2134	A	N7-C8-N9	-12.11	107.74	113.80
22	BA	1392	A	N7-C8-N9	-12.11	107.75	113.80
22	BA	603	A	N7-C8-N9	-12.10	107.75	113.80
1	AA	978	A	C5-C6-N6	12.10	133.38	123.70
22	BA	1640	A	C5-C6-N6	12.10	133.38	123.70
22	BA	1579	A	N7-C8-N9	-12.09	107.75	113.80
1	AA	729	A	C5-C6-N6	12.09	133.37	123.70
22	BA	502	A	C5-C6-N6	12.09	133.37	123.70
22	BA	2899	A	N7-C8-N9	-12.09	107.76	113.80
1	AA	602	A	N7-C8-N9	-12.09	107.76	113.80
22	BA	63	A	N7-C8-N9	-12.09	107.76	113.80
1	AA	815	A	N7-C8-N9	-12.09	107.76	113.80
1	AA	1046	A	N7-C8-N9	-12.09	107.76	113.80
1	AA	149	A	C5-C6-N6	12.08	133.37	123.70
1	AA	712	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	1815	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	2820	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	2469	A	N7-C8-N9	-12.08	107.76	113.80
1	AA	1513	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	1745	A	N7-C8-N9	-12.08	107.76	113.80
1	AA	583	A	C5-C6-N6	12.07	133.36	123.70
22	BA	1532	A	N7-C8-N9	-12.07	107.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	768	A	N7-C8-N9	-12.07	107.77	113.80
1	AA	784	A	N7-C8-N9	-12.07	107.77	113.80
1	AA	1446	A	C5-C6-N6	12.07	133.35	123.70
1	AA	533	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	160	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	2058	A	C5-C6-N6	12.06	133.35	123.70
22	BA	2154	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	2225	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	126	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	513	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	1254	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	2448	A	C5-C6-N6	12.05	133.34	123.70
22	BA	1095	A	N7-C8-N9	-12.05	107.77	113.80
1	AA	1480	A	C5-C6-N6	12.05	133.34	123.70
1	AA	547	A	N7-C8-N9	-12.05	107.78	113.80
22	BA	1189	A	N7-C8-N9	-12.05	107.78	113.80
22	BA	2163	A	N7-C8-N9	-12.05	107.78	113.80
22	BA	1453	A	N7-C8-N9	-12.04	107.78	113.80
1	AA	1410	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	2860	A	N7-C8-N9	-12.04	107.78	113.80
1	AA	1456	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	1142	A	C5-C6-N6	12.04	133.33	123.70
1	AA	131	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	501	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	1069	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	53	A	C5-C6-N6	12.04	133.33	123.70
22	BA	1321	A	C5-C6-N6	12.04	133.33	123.70
22	BA	2764	A	C5-C6-N6	12.04	133.33	123.70
1	AA	1201	A	N7-C8-N9	-12.03	107.78	113.80
22	BA	2278	A	C5-C6-N6	12.03	133.33	123.70
22	BA	2566	A	N7-C8-N9	-12.03	107.78	113.80
22	BA	2886	A	N7-C8-N9	-12.03	107.78	113.80
1	AA	1333	A	C5-C6-N6	12.03	133.32	123.70
1	AA	482	A	N7-C8-N9	-12.03	107.79	113.80
22	BA	71	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	172	A	N7-C8-N9	-12.02	107.79	113.80
1	AA	389	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	603	A	C5-C6-N6	12.02	133.32	123.70
22	BA	1384	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	2439	A	N7-C8-N9	-12.02	107.79	113.80
1	AA	622	A	C5-C6-N6	12.02	133.31	123.70
22	BA	101	A	N3-C4-C5	-12.01	118.39	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	72	A	N7-C8-N9	-12.01	107.80	113.80
1	AA	498	A	N7-C8-N9	-12.01	107.80	113.80
22	BA	990	A	N7-C8-N9	-12.01	107.80	113.80
1	AA	649	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	412	A	C5-C6-N6	12.00	133.30	123.70
1	AA	906	A	N7-C8-N9	-11.99	107.80	113.80
22	BA	670	A	C5-C6-N6	11.99	133.30	123.70
1	AA	1151	A	N7-C8-N9	-11.99	107.80	113.80
22	BA	497	A	N7-C8-N9	-11.99	107.80	113.80
1	AA	263	A	N7-C8-N9	-11.99	107.80	113.80
1	AA	1204	A	N7-C8-N9	-11.99	107.81	113.80
1	AA	1022	A	N7-C8-N9	-11.99	107.81	113.80
22	BA	627	A	N7-C8-N9	-11.99	107.81	113.80
22	BA	1505	A	N7-C8-N9	-11.98	107.81	113.80
22	BA	2418	A	N7-C8-N9	-11.97	107.81	113.80
1	AA	179	A	C5-C6-N6	11.97	133.28	123.70
22	BA	2733	A	N7-C8-N9	-11.97	107.81	113.80
1	AA	1251	A	N7-C8-N9	-11.97	107.81	113.80
22	BA	216	A	N7-C8-N9	-11.97	107.81	113.80
1	AA	1000	A	N7-C8-N9	-11.96	107.82	113.80
1	AA	1145	A	C5-C6-N6	11.96	133.27	123.70
22	BA	156	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	1854	A	N7-C8-N9	-11.97	107.82	113.80
1	AA	1493	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	1553	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	1598	A	C5-C6-N6	11.96	133.27	123.70
1	AA	889	A	C5-C6-N6	11.96	133.27	123.70
22	BA	792	A	C5-C6-N6	11.96	133.27	123.70
1	AA	1447	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	1785	A	C5-C6-N6	11.95	133.26	123.70
22	BA	2530	A	N7-C8-N9	-11.95	107.82	113.80
22	BA	1889	A	N7-C8-N9	-11.95	107.82	113.80
22	BA	2288	A	N7-C8-N9	-11.95	107.83	113.80
1	AA	172	A	N7-C8-N9	-11.95	107.83	113.80
1	AA	687	A	C5-C6-N6	11.94	133.26	123.70
22	BA	1156	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	199	A	C5-C6-N6	11.94	133.25	123.70
22	BA	2541	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	1272	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	752	A	N9-C4-C5	11.94	110.57	105.80
22	BA	2386	A	N7-C8-N9	-11.94	107.83	113.80
1	AA	1042	A	N7-C8-N9	-11.93	107.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	374	A	N7-C8-N9	-11.93	107.83	113.80
22	BA	2439	A	C5-C6-N6	11.93	133.25	123.70
22	BA	936	A	N7-C8-N9	-11.93	107.83	113.80
1	AA	759	A	C5-C6-N6	11.93	133.24	123.70
1	AA	1150	A	N7-C8-N9	-11.93	107.83	113.80
22	BA	522	A	N3-C4-C5	-11.93	118.45	126.80
1	AA	909	A	C5-C6-N6	11.93	133.24	123.70
22	BA	161	A	N7-C8-N9	-11.93	107.84	113.80
22	BA	256	A	N7-C8-N9	-11.93	107.84	113.80
1	AA	298	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	1918	A	N7-C8-N9	-11.92	107.84	113.80
1	AA	1269	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	1608	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	2392	A	C5-C6-N6	11.92	133.24	123.70
23	BB	50	A	N7-C8-N9	-11.92	107.84	113.80
1	AA	2	A	N7-C8-N9	-11.91	107.84	113.80
1	AA	50	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	10	A	N7-C8-N9	-11.91	107.85	113.80
22	BA	1713	A	N7-C8-N9	-11.91	107.85	113.80
22	BA	1175	A	N3-C4-C5	-11.90	118.47	126.80
1	AA	51	A	N7-C8-N9	-11.90	107.85	113.80
22	BA	1916	A	C5-C6-N6	11.90	133.22	123.70
22	BA	1952	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	892	A	N7-C8-N9	-11.90	107.85	113.80
22	BA	1966	A	N7-C8-N9	-11.89	107.85	113.80
1	AA	794	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	2850	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	7	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	28	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	1092	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	1248	A	C5-C6-N6	11.88	133.21	123.70
22	BA	1253	A	C5-C6-N6	11.88	133.20	123.70
22	BA	1431	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	1772	A	C5-C6-N6	11.88	133.20	123.70
1	AA	26	A	N7-C8-N9	-11.87	107.86	113.80
1	AA	878	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	2227	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	2776	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	925	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	1571	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	1755	A	C5-C6-N6	11.87	133.20	123.70
22	BA	2406	A	C5-C6-N6	11.87	133.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1271	A	N7-C8-N9	-11.87	107.87	113.80
22	BA	1237	A	C5-C6-N6	11.87	133.19	123.70
22	BA	227	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	1928	A	C5-C6-N6	11.86	133.19	123.70
1	AA	16	A	N7-C8-N9	-11.86	107.87	113.80
1	AA	937	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	1021	A	C5-C6-N6	11.86	133.19	123.70
22	BA	2634	A	N7-C8-N9	-11.86	107.87	113.80
1	AA	831	A	N7-C8-N9	-11.85	107.87	113.80
22	BA	947	A	N7-C8-N9	-11.85	107.87	113.80
22	BA	1810	A	N3-C4-C5	-11.85	118.50	126.80
22	BA	2346	A	C5-C6-N6	11.85	133.18	123.70
1	AA	1289	A	N7-C8-N9	-11.85	107.88	113.80
1	AA	98	A	N3-C4-C5	-11.85	118.51	126.80
1	AA	532	A	N7-C8-N9	-11.85	107.88	113.80
22	BA	142	A	N7-C8-N9	-11.85	107.88	113.80
22	BA	401	A	N7-C8-N9	-11.85	107.88	113.80
1	AA	430	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	74	A	C5-C6-N6	11.84	133.18	123.70
22	BA	233	A	N7-C8-N9	-11.84	107.88	113.80
1	AA	303	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	340	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	6	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	2872	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	439	A	N7-C8-N9	-11.83	107.88	113.80
22	BA	505	A	N7-C8-N9	-11.83	107.89	113.80
22	BA	127	A	N7-C8-N9	-11.83	107.89	113.80
55	B8	58	A	N7-C8-N9	-11.83	107.89	113.80
1	AA	74	A	C5-C6-N6	11.82	133.16	123.70
22	BA	1336	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	1635	A	C5-C6-N6	11.82	133.16	123.70
1	AA	129	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	2679	A	N3-C4-C5	-11.82	118.53	126.80
1	AA	648	A	N7-C8-N9	-11.81	107.89	113.80
22	BA	190	A	C5-C6-N6	11.80	133.14	123.70
22	BA	661	A	C5-C6-N6	11.80	133.14	123.70
1	AA	621	A	C5-C6-N6	11.80	133.14	123.70
1	AA	1319	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	1302	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	1395	A	C5-C6-N6	11.79	133.13	123.70
1	AA	238	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	1285	A	C5-C6-N6	11.79	133.13	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1385	A	C5-C6-N6	11.79	133.13	123.70
22	BA	2572	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	1067	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1998	A	C5-C6-N6	11.79	133.13	123.70
1	AA	179	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1698	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	332	A	C5-C6-N6	11.78	133.13	123.70
22	BA	2476	A	C5-C6-N6	11.79	133.13	123.70
1	AA	1171	A	N3-C4-C5	-11.78	118.55	126.80
22	BA	74	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	532	A	C5-C6-N6	11.78	133.13	123.70
22	BA	1677	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	21	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	1783	A	C5-C6-N6	11.78	133.12	123.70
22	BA	181	A	C5-C6-N6	11.78	133.12	123.70
22	BA	342	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	2547	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	152	A	N7-C8-N9	-11.77	107.91	113.80
22	BA	792	A	N7-C8-N9	-11.77	107.91	113.80
22	BA	1050	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1155	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1353	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1701	A	C5-C6-N6	11.77	133.11	123.70
1	AA	487	A	N7-C8-N9	-11.76	107.92	113.80
1	AA	681	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	332	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	718	A	C5-C6-N6	11.76	133.11	123.70
22	BA	2430	A	N1-C2-N3	-11.76	123.42	129.30
22	BA	1028	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	1936	A	N3-C4-C5	-11.75	118.57	126.80
22	BA	1169	A	N7-C8-N9	-11.75	107.92	113.80
22	BA	2158	A	C5-C6-N6	11.75	133.10	123.70
1	AA	807	A	C5-C6-N6	11.75	133.10	123.70
22	BA	1970	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	509	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	1110	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	368	A	N7-C8-N9	-11.73	107.93	113.80
22	BA	371	A	C5-C6-N6	11.73	133.09	123.70
22	BA	1640	A	N7-C8-N9	-11.73	107.93	113.80
22	BA	2450	A	N7-C8-N9	-11.73	107.94	113.80
23	BB	104	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	2171	A	N7-C8-N9	-11.72	107.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1014	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	1332	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	1142	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	38	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	181	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	2267	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	496	A	C5-C6-N6	11.71	133.07	123.70
22	BA	1247	A	C5-C6-N6	11.72	133.07	123.70
1	AA	715	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	915	A	C5-C6-N6	11.71	133.07	123.70
22	BA	482	A	N1-C6-N6	-11.72	111.57	118.60
22	BA	981	A	C5-C6-N6	11.72	133.07	123.70
1	AA	456	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	412	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	599	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	1515	A	N7-C8-N9	-11.71	107.94	113.80
23	BB	78	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	1286	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	181	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	1069	A	C5-C6-N6	11.71	133.07	123.70
22	BA	1701	A	N7-C8-N9	-11.71	107.95	113.80
1	AA	382	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	73	A	C5-C6-N6	11.71	133.06	123.70
22	BA	788	A	C5-C6-N6	11.71	133.06	123.70
22	BA	1155	A	C5-C6-N6	11.71	133.06	123.70
22	BA	2577	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	2711	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	2632	A	C5-C6-N6	11.70	133.06	123.70
22	BA	173	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	2369	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	1535	A	C5-C6-N6	11.69	133.06	123.70
22	BA	2037	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	1088	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	2205	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	1447	A	C5-C6-N6	11.69	133.05	123.70
22	BA	118	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	1470	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	621	A	N7-C8-N9	-11.69	107.96	113.80
55	B8	73	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	149	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	452	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	1170	A	N7-C8-N9	-11.68	107.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	429	A	C5-C6-N6	11.68	133.05	123.70
22	BA	1650	A	C5-C6-N6	11.68	133.05	123.70
1	AA	1254	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	1246	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	573	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	670	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	1641	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	2497	A	N3-C4-C5	-11.68	118.62	126.80
1	AA	68	G	C4-N9-C1'	11.68	141.68	126.50
22	BA	2309	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	1483	A	N7-C8-N9	-11.67	107.96	113.80
22	BA	716	A	N7-C8-N9	-11.67	107.97	113.80
22	BA	1057	A	C5-C6-N6	11.67	133.03	123.70
22	BA	91	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	907	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	1157	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	139	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	443	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	1853	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1236	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	2564	A	C5-C6-N6	11.65	133.02	123.70
1	AA	914	A	C5-C6-N6	11.65	133.02	123.70
22	BA	1029	A	N7-C8-N9	-11.65	107.98	113.80
22	BA	346	A	N7-C8-N9	-11.65	107.98	113.80
22	BA	1262	A	C5-C6-N6	11.65	133.02	123.70
1	AA	160	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	1188	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	917	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	1165	A	C5-C6-N6	11.64	133.01	123.70
22	BA	2268	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	2778	A	C5-C6-N6	11.64	133.01	123.70
22	BA	2095	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	2882	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	559	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	1226	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	1311	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	2052	A	N3-C4-C5	-11.63	118.66	126.80
22	BA	2434	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	397	A	N3-C4-C5	-11.62	118.67	126.80
1	AA	642	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1322	A	C5-C6-N6	11.62	133.00	123.70
22	BA	2147	A	N7-C8-N9	-11.62	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1319	A	C5-C6-N6	11.62	132.99	123.70
22	BA	2169	A	C5-C6-N6	11.62	132.99	123.70
1	AA	1169	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	231	A	N3-C4-C5	-11.62	118.67	126.80
1	AA	746	A	N3-C4-C5	-11.61	118.67	126.80
1	AA	1446	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1176	A	N7-C8-N9	-11.61	107.99	113.80
22	BA	1129	A	C5-C6-N6	11.61	132.99	123.70
22	BA	1522	A	C5-C6-N6	11.61	132.98	123.70
22	BA	1650	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	2734	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	2799	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	101	A	C5-N7-C8	11.60	109.70	103.90
55	B8	51	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	977	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	1008	A	C5-C6-N6	11.60	132.98	123.70
1	AA	845	A	C5-C6-N6	11.60	132.98	123.70
22	BA	270	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	2451	A	C5-C6-N6	11.59	132.97	123.70
55	B8	21	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	1492	A	C5-C6-N6	11.59	132.97	123.70
22	BA	89	A	C5-C6-N6	11.59	132.97	123.70
22	BA	84	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	1089	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1022	A	C5-C6-N6	11.58	132.96	123.70
22	BA	800	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	781	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	983	A	N7-C8-N9	-11.57	108.01	113.80
22	BA	1808	A	N7-C8-N9	-11.57	108.01	113.80
22	BA	345	A	C5-C6-N6	11.57	132.96	123.70
22	BA	223	A	C5-C6-N6	11.57	132.96	123.70
22	BA	1126	A	C5-C6-N6	11.57	132.96	123.70
22	BA	2267	A	N3-C4-C5	-11.57	118.70	126.80
22	BA	2750	A	C5-C6-N6	11.57	132.96	123.70
22	BA	973	A	C5-C6-N6	11.57	132.95	123.70
22	BA	1502	A	N7-C8-N9	-11.57	108.02	113.80
55	B8	38	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	553	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	391	A	N7-C8-N9	-11.56	108.02	113.80
23	BB	109	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	592	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	1705	A	N7-C8-N9	-11.55	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	65	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1167	A	C5-C6-N6	11.55	132.94	123.70
1	AA	1288	A	C5-C6-N6	11.55	132.94	123.70
22	BA	2314	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	325	A	C5-C6-N6	11.55	132.94	123.70
1	AA	728	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	55	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1434	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	1759	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	129	A	C5-C6-N6	11.54	132.93	123.70
22	BA	1285	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	16	A	C5-C6-N6	11.53	132.93	123.70
1	AA	99	C	N3-C2-O2	-11.53	113.83	121.90
22	BA	644	A	N3-C4-C5	-11.53	118.73	126.80
22	BA	1630	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	2070	A	C5-C6-N6	11.53	132.93	123.70
22	BA	2542	A	C5-C6-N6	11.53	132.93	123.70
22	BA	1244	A	C5-C6-N6	11.53	132.92	123.70
1	AA	1287	A	C5-C6-N6	11.53	132.92	123.70
22	BA	404	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	556	A	C5-C6-N6	11.52	132.92	123.70
22	BA	2660	A	C5-C6-N6	11.52	132.92	123.70
22	BA	1274	A	N7-C8-N9	-11.52	108.04	113.80
54	B7	9	A	C5-C6-N6	11.52	132.92	123.70
22	BA	613	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	430	A	C5-C6-N6	11.52	132.91	123.70
22	BA	503	A	N3-C4-C5	-11.52	118.74	126.80
22	BA	782	A	C5-C6-N6	11.52	132.91	123.70
22	BA	2119	A	N7-C8-N9	-11.52	108.04	113.80
23	BB	59	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	2761	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	572	A	N3-C4-C5	-11.51	118.74	126.80
55	B8	14	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	192	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	743	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1534	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	1020	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1689	A	C5-C6-N6	11.50	132.90	123.70
1	AA	635	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	919	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1900	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	205	A	N7-C8-N9	-11.50	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1494	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1586	A	C5-C6-N6	11.50	132.90	123.70
22	BA	223	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	787	A	C5-C6-N6	11.49	132.90	123.70
22	BA	2058	A	N7-C8-N9	-11.49	108.05	113.80
22	BA	2212	A	N7-C8-N9	-11.49	108.06	113.80
23	BB	53	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	563	A	N3-C4-C5	-11.49	118.76	126.80
1	AA	1157	A	C5-C6-N6	11.49	132.89	123.70
1	AA	676	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	743	A	N7-C8-N9	-11.49	108.06	113.80
22	BA	1655	A	C5-C6-N6	11.49	132.89	123.70
22	BA	2541	A	C5-C6-N6	11.49	132.89	123.70
1	AA	768	A	C5-C6-N6	11.48	132.89	123.70
22	BA	590	A	C5-C6-N6	11.48	132.89	123.70
1	AA	913	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	914	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	56	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1143	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1525	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1342	A	C5-C6-N6	11.48	132.88	123.70
22	BA	203	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	613	A	C5-C6-N6	11.47	132.88	123.70
22	BA	945	A	N3-C4-C5	-11.47	118.77	126.80
22	BA	182	A	C5-C6-N6	11.47	132.88	123.70
1	AA	607	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	648	A	C5-C6-N6	11.47	132.87	123.70
22	BA	2170	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	533	A	N3-C4-C5	-11.47	118.77	126.80
1	AA	1055	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	423	A	C5-C6-N6	11.46	132.87	123.70
22	BA	1572	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	1871	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	246	A	C5-C6-N6	11.46	132.87	123.70
1	AA	595	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	753	A	C5-C6-N6	11.46	132.86	123.70
22	BA	324	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	1433	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	423	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	250	A	C5-C6-N6	11.45	132.86	123.70
22	BA	2033	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	2117	A	N7-C8-N9	-11.45	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	44	A	C5-C6-N6	11.45	132.86	123.70
1	AA	968	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	1885	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1375	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	49	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	195	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	344	A	C5-C6-N6	11.44	132.85	123.70
1	AA	33	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2173	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2800	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1239	A	C5-C6-N6	11.43	132.85	123.70
22	BA	1284	A	C5-C6-N6	11.43	132.85	123.70
22	BA	1918	A	C5-C6-N6	11.43	132.85	123.70
22	BA	415	A	N3-C4-C5	-11.43	118.80	126.80
22	BA	574	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	958	A	C5-C6-N6	11.43	132.84	123.70
22	BA	2094	A	N7-C8-N9	-11.43	108.09	113.80
22	BA	1133	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	1350	A	N7-C8-N9	-11.43	108.09	113.80
22	BA	415	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	715	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1387	A	N7-C8-N9	-11.42	108.09	113.80
23	BB	52	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1035	A	N3-C4-C5	-11.42	118.80	126.80
22	BA	477	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	73	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1098	A	C5-C6-N6	11.42	132.83	123.70
22	BA	1262	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	226	A	N3-C4-C5	-11.41	118.81	126.80
1	AA	977	A	C5-C6-N6	11.41	132.83	123.70
22	BA	231	A	N7-C8-N9	-11.41	108.09	113.80
22	BA	866	A	C5-C6-N6	11.41	132.83	123.70
22	BA	165	A	C5-C6-N6	11.41	132.83	123.70
22	BA	483	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	459	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	1145	A	N7-C8-N9	-11.41	108.10	113.80
1	AA	197	A	C5-C6-N6	11.41	132.83	123.70
22	BA	119	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	1549	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	144	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	547	A	C5-C6-N6	11.40	132.82	123.70
22	BA	1127	A	N7-C8-N9	-11.40	108.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2406	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	2639	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	1289	A	C5-C6-N6	11.40	132.82	123.70
22	BA	616	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	1070	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	523	A	N7-C8-N9	-11.39	108.10	113.80
22	BA	920	A	N7-C8-N9	-11.39	108.10	113.80
22	BA	892	A	C5-C6-N6	11.39	132.81	123.70
22	BA	1269	A	N3-C4-C5	-11.39	118.82	126.80
1	AA	174	A	C5-C6-N6	11.39	132.81	123.70
22	BA	2225	A	C5-C6-N6	11.39	132.81	123.70
1	AA	532	A	C5-C6-N6	11.39	132.81	123.70
1	AA	1431	A	C5-C6-N6	11.39	132.81	123.70
23	BB	52	A	C5-C6-N6	11.39	132.81	123.70
22	BA	2176	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2314	A	C5-C6-N6	11.39	132.81	123.70
22	BA	322	A	C5-C6-N6	11.39	132.81	123.70
22	BA	2778	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	262	A	N7-C8-N9	-11.38	108.11	113.80
22	BA	988	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	814	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	595	A	C5-C6-N6	11.38	132.80	123.70
1	AA	1362	A	C5-C6-N6	11.38	132.80	123.70
22	BA	996	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1101	A	C5-C6-N6	11.37	132.80	123.70
1	AA	1465	A	C5-C6-N6	11.38	132.80	123.70
22	BA	821	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	1084	A	N7-C8-N9	-11.37	108.12	113.80
22	BA	2114	A	N3-C4-C5	-11.37	118.84	126.80
22	BA	2741	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	101	A	N3-C4-C5	-11.37	118.84	126.80
22	BA	1819	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	116	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	189	A	C5-C6-N6	11.37	132.79	123.70
1	AA	189	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	263	A	C5-C6-N6	11.36	132.79	123.70
1	AA	1246	A	C5-C6-N6	11.36	132.79	123.70
22	BA	207	A	C5-C6-N6	11.36	132.79	123.70
22	BA	2273	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	2448	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	2530	A	C5-C6-N6	11.36	132.79	123.70
1	AA	1012	A	N7-C8-N9	-11.36	108.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	311	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	1036	A	C5-C6-N6	11.35	132.78	123.70
22	BA	155	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	196	A	N3-C4-C5	-11.35	118.86	126.80
22	BA	1735	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	860	A	C5-C6-N6	11.35	132.78	123.70
22	BA	1912	A	N7-C8-N9	-11.35	108.13	113.80
22	BA	2199	A	C5-C6-N6	11.34	132.78	123.70
22	BA	2856	A	C5-C6-N6	11.34	132.78	123.70
22	BA	1780	A	C5-C6-N6	11.34	132.77	123.70
1	AA	946	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	300	A	C5-C6-N6	11.34	132.77	123.70
22	BA	643	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	574	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1500	A	C5-C6-N6	11.34	132.77	123.70
22	BA	1134	A	N3-C4-C5	-11.34	118.87	126.80
1	AA	412	A	C5-C6-N6	11.33	132.77	123.70
55	B8	73	A	C5-C6-N6	11.33	132.77	123.70
1	AA	1374	A	N7-C8-N9	-11.33	108.13	113.80
22	BA	1551	A	N7-C8-N9	-11.33	108.13	113.80
22	BA	2163	A	C5-C6-N6	11.33	132.76	123.70
22	BA	1938	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	1349	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	2298	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	2311	A	C5-C6-N6	11.33	132.76	123.70
22	BA	2727	A	N3-C4-C5	-11.33	118.87	126.80
1	AA	223	A	C5-C6-N6	11.32	132.76	123.70
1	AA	1324	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	1960	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	402	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	816	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	742	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	794	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	1590	A	N7-C8-N9	-11.32	108.14	113.80
23	BB	39	A	C5-C6-N6	11.32	132.75	123.70
1	AA	1500	A	N7-C8-N9	-11.31	108.14	113.80
22	BA	1815	A	C5-C6-N6	11.31	132.75	123.70
22	BA	2814	A	C5-C6-N6	11.31	132.75	123.70
1	AA	609	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	695	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	845	A	N7-C8-N9	-11.31	108.14	113.80
55	B8	6	A	N7-C8-N9	-11.31	108.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	59	A	N7-C8-N9	-11.31	108.15	113.80
22	BA	752	A	N3-C4-C5	-11.31	118.88	126.80
22	BA	2267	A	C5-C6-N6	11.31	132.75	123.70
1	AA	270	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	949	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	1252	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	2826	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	1146	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1468	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1545	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	696	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	892	A	C5-C6-N6	11.30	132.74	123.70
1	AA	969	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1437	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	2247	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1919	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	938	A	N3-C4-C5	-11.29	118.90	126.80
1	AA	964	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	960	A	N3-C4-C5	-11.29	118.90	126.80
22	BA	2270	A	C5-C6-N6	11.29	132.73	123.70
23	BB	29	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	975	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	2425	A	N7-C8-N9	-11.28	108.16	113.80
23	BB	78	A	C5-C6-N6	11.28	132.73	123.70
1	AA	873	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1276	A	C5-C6-N6	11.28	132.72	123.70
22	BA	1548	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1342	A	N7-C8-N9	-11.28	108.16	113.80
55	B8	41	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	6	A	C5-C6-N6	11.27	132.72	123.70
22	BA	432	A	C5-C6-N6	11.27	132.72	123.70
22	BA	472	A	C5-C6-N6	11.27	132.72	123.70
22	BA	479	A	C5-C6-N6	11.27	132.72	123.70
22	BA	1054	A	N3-C4-C5	-11.27	118.91	126.80
22	BA	1978	A	N7-C8-N9	-11.27	108.17	113.80
1	AA	364	A	C5-C6-N6	11.27	132.71	123.70
22	BA	1027	A	C8-N9-C4	11.27	110.31	105.80
22	BA	2274	A	C5-C6-N6	11.27	132.71	123.70
23	BB	46	A	C5-C6-N6	11.27	132.71	123.70
1	AA	81	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	975	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	666	A	C5-C6-N6	11.26	132.71	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1048	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	315	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	363	A	C5-C6-N6	11.26	132.71	123.70
1	AA	1130	A	C5-C6-N6	11.26	132.71	123.70
22	BA	1801	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	2757	A	N3-C4-C5	-11.26	118.92	126.80
1	AA	174	A	N3-C4-C5	-11.26	118.92	126.80
1	AA	1248	A	N7-C8-N9	-11.25	108.17	113.80
1	AA	1502	A	C5-C6-N6	11.25	132.70	123.70
22	BA	2311	A	N7-C8-N9	-11.25	108.18	113.80
1	AA	1042	A	C5-C6-N6	11.25	132.70	123.70
1	AA	1531	A	C5-C6-N6	11.24	132.69	123.70
1	AA	1288	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	1505	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1545	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2054	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	2662	A	N3-C4-C5	-11.24	118.93	126.80
22	BA	1095	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1544	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	2014	A	C5-C6-N6	11.24	132.69	123.70
22	BA	402	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2352	A	C5-C6-N6	11.24	132.69	123.70
1	AA	288	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	478	A	N7-C8-N9	-11.23	108.18	113.80
22	BA	1134	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	816	A	C5-C6-N6	11.23	132.69	123.70
22	BA	219	A	C5-C6-N6	11.23	132.69	123.70
22	BA	1899	A	C5-C6-N6	11.23	132.68	123.70
22	BA	783	A	C5-C6-N6	11.23	132.68	123.70
22	BA	2317	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	2736	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	362	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	2297	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	514	A	C5-C6-N6	11.22	132.67	123.70
1	AA	325	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	1744	A	C5-C6-N6	11.22	132.67	123.70
22	BA	2198	A	N7-C8-N9	-11.21	108.19	113.80
22	BA	2734	A	C5-C6-N6	11.21	132.67	123.70
22	BA	2051	A	N3-C4-C5	-11.21	118.96	126.80
22	BA	2660	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	1111	A	C5-C6-N6	11.20	132.66	123.70
22	BA	668	A	C5-C6-N6	11.20	132.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	905	A	C5-C6-N6	11.20	132.66	123.70
1	AA	274	A	C5-C6-N6	11.20	132.66	123.70
22	BA	1678	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2879	A	N3-C4-C5	-11.20	118.96	126.80
22	BA	203	A	C5-C6-N6	11.20	132.66	123.70
1	AA	8	A	C5-C6-N6	11.20	132.66	123.70
1	AA	432	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	1569	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2727	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2879	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	1690	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	131	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	504	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	1665	A	C5-C6-N6	11.19	132.65	123.70
22	BA	2753	A	N7-C8-N9	-11.19	108.20	113.80
1	AA	1197	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	2433	A	N7-C8-N9	-11.19	108.21	113.80
1	AA	344	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	1552	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	1919	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1928	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	1637	A	N7-C8-N9	-11.19	108.21	113.80
1	AA	3	A	N7-C8-N9	-11.18	108.21	113.80
55	B8	21	A	C5-C6-N6	11.18	132.65	123.70
1	AA	451	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	38	A	C5-C6-N6	11.18	132.64	123.70
22	BA	735	A	C5-C6-N6	11.18	132.64	123.70
22	BA	825	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	1304	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1495	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1668	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	204	A	N7-C8-N9	-11.17	108.22	113.80
22	BA	1913	A	C5-C6-N6	11.17	132.64	123.70
22	BA	2810	A	C5-C6-N6	11.17	132.64	123.70
22	BA	693	A	C5-C6-N6	11.17	132.63	123.70
22	BA	735	A	N7-C8-N9	-11.17	108.22	113.80
22	BA	2453	A	N3-C4-C5	-11.17	118.98	126.80
22	BA	1142	A	N3-C4-C5	-11.16	118.98	126.80
1	AA	1257	A	C5-C6-N6	11.16	132.63	123.70
22	BA	783	A	N3-C4-C5	-11.16	118.99	126.80
22	BA	1403	A	C5-C6-N6	11.16	132.63	123.70
22	BA	1786	A	C5-C6-N6	11.16	132.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2134	A	C5-C6-N6	11.16	132.63	123.70
1	AA	7	A	C5-C6-N6	11.16	132.63	123.70
1	AA	32	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	861	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	505	A	C5-C6-N6	11.16	132.63	123.70
22	BA	556	A	N7-C8-N9	-11.16	108.22	113.80
23	BB	50	A	C5-C6-N6	11.16	132.62	123.70
22	BA	2706	A	C5-C6-N6	11.15	132.62	123.70
1	AA	865	A	N3-C4-C5	-11.15	118.99	126.80
1	AA	1396	A	N3-C4-C5	-11.15	118.99	126.80
22	BA	1665	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	196	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1287	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	1477	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1067	A	C5-C6-N6	11.15	132.62	123.70
1	AA	1111	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	329	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	704	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	1360	A	C5-C6-N6	11.14	132.62	123.70
22	BA	1746	A	C5-C6-N6	11.14	132.61	123.70
22	BA	2448	A	N3-C4-C5	-11.14	119.00	126.80
22	BA	1084	A	C5-C6-N6	11.14	132.61	123.70
22	BA	2158	A	N7-C8-N9	-11.14	108.23	113.80
55	B8	42	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	1269	A	C5-C6-N6	11.14	132.61	123.70
22	BA	2873	A	C5-C6-N6	11.14	132.61	123.70
1	AA	1204	A	C5-C6-N6	11.13	132.60	123.70
22	BA	1525	A	C5-C6-N6	11.13	132.60	123.70
1	AA	959	A	N7-C8-N9	-11.13	108.24	113.80
1	AA	478	A	C5-C6-N6	11.12	132.60	123.70
22	BA	1876	A	C5-C6-N6	11.13	132.60	123.70
22	BA	2418	A	C5-C6-N6	11.13	132.60	123.70
22	BA	1133	A	N3-C4-C5	-11.12	119.01	126.80
22	BA	2900	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	1453	A	C5-C6-N6	11.12	132.60	123.70
22	BA	988	A	C5-C6-N6	11.12	132.60	123.70
23	BB	45	A	C5-C6-N6	11.12	132.60	123.70
22	BA	2518	A	N3-C4-C5	-11.12	119.02	126.80
1	AA	412	A	N7-C8-N9	-11.11	108.24	113.80
1	AA	1019	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	764	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1689	A	N7-C8-N9	-11.11	108.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1853	A	C5-C6-N6	11.11	132.59	123.70
22	BA	2837	A	N7-C8-N9	-11.11	108.25	113.80
1	AA	109	A	C5-C6-N6	11.11	132.59	123.70
22	BA	94	A	C5-C6-N6	11.11	132.59	123.70
22	BA	2346	A	N7-C8-N9	-11.11	108.25	113.80
1	AA	1299	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	1553	A	C5-C6-N6	11.10	132.58	123.70
22	BA	1610	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	2062	A	N7-C8-N9	-11.10	108.25	113.80
1	AA	663	A	N7-C8-N9	-11.10	108.25	113.80
1	AA	313	A	N3-C4-C5	-11.09	119.03	126.80
22	BA	730	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	933	A	N3-C4-C5	-11.09	119.03	126.80
1	AA	563	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	142	A	C5-C6-N6	11.09	132.57	123.70
22	BA	165	A	N7-C8-N9	-11.09	108.26	113.80
1	AA	1044	A	N7-C8-N9	-11.09	108.26	113.80
22	BA	1912	A	C5-C6-N6	11.09	132.57	123.70
1	AA	55	A	N3-C4-C5	-11.08	119.04	126.80
22	BA	706	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	864	A	C5-C6-N6	11.08	132.57	123.70
1	AA	1250	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	447	A	C5-C6-N6	11.08	132.57	123.70
22	BA	1544	A	C5-C6-N6	11.08	132.57	123.70
22	BA	428	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	2358	A	C5-C6-N6	11.08	132.56	123.70
1	AA	315	A	C5-C6-N6	11.08	132.56	123.70
22	BA	1085	A	C5-C6-N6	11.08	132.56	123.70
22	BA	2587	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	44	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	338	A	N7-C8-N9	-11.08	108.26	113.80
23	BB	94	A	C5-C6-N6	11.08	132.56	123.70
22	BA	621	A	C5-C6-N6	11.07	132.56	123.70
1	AA	908	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	1287	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	2082	A	N7-C8-N9	-11.07	108.26	113.80
54	B7	9	A	N3-C4-C5	-11.07	119.05	126.80
1	AA	466	A	C5-C6-N6	11.07	132.56	123.70
22	BA	262	A	C5-C6-N6	11.07	132.56	123.70
22	BA	1321	A	N3-C4-C5	-11.07	119.05	126.80
55	B8	14	A	C5-C6-N6	11.07	132.56	123.70
1	AA	706	A	N7-C8-N9	-11.07	108.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1339	A	N7-C8-N9	-11.07	108.27	113.80
1	AA	560	A	C5-C6-N6	11.06	132.55	123.70
22	BA	673	C	C2-N3-C4	-11.06	114.37	119.90
1	AA	819	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	448	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	2322	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	313	A	N7-C8-N9	-11.05	108.27	113.80
1	AA	1005	A	C5-C6-N6	11.05	132.54	123.70
22	BA	654	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	742	A	N3-C4-C5	-11.05	119.06	126.80
22	BA	1829	A	C5-C6-N6	11.05	132.54	123.70
1	AA	60	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	1916	A	N7-C8-N9	-11.05	108.27	113.80
1	AA	629	A	N7-C8-N9	-11.05	108.28	113.80
22	BA	1395	A	N7-C8-N9	-11.05	108.28	113.80
22	BA	1427	A	C5-C6-N6	11.05	132.54	123.70
22	BA	1664	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	1876	A	N7-C8-N9	-11.05	108.28	113.80
1	AA	864	A	N7-C8-N9	-11.05	108.28	113.80
23	BB	45	A	N3-C4-C5	-11.05	119.07	126.80
22	BA	1111	A	C5-C6-N6	11.04	132.54	123.70
1	AA	151	A	C5-C6-N6	11.04	132.53	123.70
1	AA	309	A	C5-C6-N6	11.04	132.53	123.70
1	AA	363	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	44	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1819	A	N3-C4-C5	-11.04	119.07	126.80
1	AA	1004	A	C5-C6-N6	11.04	132.53	123.70
1	AA	1216	A	N7-C8-N9	-11.04	108.28	113.80
1	AA	1285	A	C5-C6-N6	11.04	132.53	123.70
22	BA	761	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1246	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	1899	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1970	A	C5-C6-N6	11.04	132.53	123.70
22	BA	1803	A	C5-C6-N6	11.04	132.53	123.70
23	BB	94	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	1048	A	C5-C6-N6	11.03	132.53	123.70
1	AA	109	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	750	A	N3-C4-C5	-11.03	119.08	126.80
22	BA	1383	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	2169	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	2590	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	439	A	N3-C4-C5	-11.03	119.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	300	A	N3-C4-C5	-11.03	119.08	126.80
22	BA	226	A	C5-C6-N6	11.03	132.52	123.70
22	BA	616	A	N3-C4-C5	-11.03	119.08	126.80
1	AA	630	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	1359	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	1096	A	C5-C6-N6	11.02	132.52	123.70
22	BA	1969	A	N7-C8-N9	-11.02	108.29	113.80
1	AA	19	A	N3-C4-C5	-11.02	119.09	126.80
1	AA	802	A	C5-C6-N6	11.02	132.52	123.70
1	AA	1374	A	C5-C6-N6	11.02	132.51	123.70
23	BB	94	A	N3-C4-C5	-11.02	119.09	126.80
22	BA	1032	A	C5-C6-N6	11.02	132.51	123.70
22	BA	2748	A	N7-C8-N9	-11.02	108.29	113.80
1	AA	1363	A	N3-C4-C5	-11.02	119.09	126.80
22	BA	182	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	2386	A	C5-C6-N6	11.02	132.51	123.70
1	AA	465	A	N7-C8-N9	-11.01	108.29	113.80
1	AA	190	A	N3-C4-C5	-11.01	119.09	126.80
22	BA	2482	A	C5-C6-N6	11.01	132.51	123.70
22	BA	675	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	928	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	1260	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	1328	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	1634	A	C5-C6-N6	11.00	132.50	123.70
22	BA	2317	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	1205	A	N7-C8-N9	-11.00	108.30	113.80
23	BB	45	A	N7-C8-N9	-11.00	108.30	113.80
1	AA	195	A	C5-C6-N6	11.00	132.50	123.70
22	BA	330	A	N7-C8-N9	-11.00	108.30	113.80
1	AA	1092	A	C5-C6-N6	11.00	132.50	123.70
22	BA	2534	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	918	A	C5-C6-N6	10.99	132.50	123.70
22	BA	454	A	C5-C6-N6	10.99	132.49	123.70
22	BA	802	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	2135	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1551	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	2060	A	C5-C6-N6	10.99	132.49	123.70
22	BA	345	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	716	A	C5-C6-N6	10.98	132.49	123.70
22	BA	1365	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	637	A	C5-C6-N6	10.98	132.49	123.70
22	BA	1264	A	N7-C8-N9	-10.98	108.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1387	A	N3-C4-C5	-10.98	119.11	126.80
22	BA	2635	A	C5-C6-N6	10.98	132.49	123.70
55	B8	69	A	N7-C8-N9	-10.98	108.31	113.80
1	AA	1201	A	N3-C4-C5	-10.98	119.12	126.80
22	BA	1067	A	C5-C6-N6	10.98	132.48	123.70
1	AA	1	A	N7-C8-N9	-10.97	108.31	113.80
1	AA	19	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	330	A	N3-C4-C5	-10.97	119.12	126.80
1	AA	466	A	N3-C4-C5	-10.96	119.12	126.80
55	B8	42	A	C5-C6-N6	10.96	132.47	123.70
1	AA	53	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	118	A	C5-C6-N6	10.96	132.47	123.70
1	AA	749	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	1503	A	C5-C6-N6	10.96	132.47	123.70
22	BA	404	A	C5-C6-N6	10.96	132.47	123.70
22	BA	676	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1877	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	2534	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1322	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	2309	A	C5-C6-N6	10.95	132.46	123.70
22	BA	2765	A	N7-C8-N9	-10.95	108.32	113.80
23	BB	108	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	310	A	C5-C6-N6	10.95	132.46	123.70
22	BA	322	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	1495	A	N7-C8-N9	-10.95	108.33	113.80
1	AA	901	A	N3-C4-C5	-10.95	119.14	126.80
22	BA	1010	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	2199	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	706	A	N3-C4-C5	-10.94	119.14	126.80
55	B8	38	A	C5-C6-N6	10.94	132.45	123.70
23	BB	73	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	900	A	C5-C6-N6	10.93	132.45	123.70
1	AA	1102	A	N3-C4-C5	-10.93	119.15	126.80
22	BA	146	A	N7-C8-N9	-10.93	108.33	113.80
55	B8	66	A	N7-C8-N9	-10.93	108.33	113.80
22	BA	1597	A	N3-C4-C5	-10.93	119.15	126.80
22	BA	2097	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	655	A	N7-C8-N9	-10.93	108.34	113.80
22	BA	2738	A	C5-C6-N6	10.93	132.44	123.70
22	BA	2851	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	1225	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	2013	A	C5-C6-N6	10.92	132.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	673	A	N7-C8-N9	-10.92	108.34	113.80
1	AA	729	A	N7-C8-N9	-10.92	108.34	113.80
1	AA	1274	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	917	A	C5-C6-N6	10.92	132.43	123.70
22	BA	2003	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	563	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1717	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1791	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1876	A	N3-C4-C5	-10.91	119.16	126.80
1	AA	461	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	1021	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	84	A	C5-C6-N6	10.91	132.43	123.70
22	BA	2813	A	C5-C6-N6	10.91	132.43	123.70
22	BA	345	A	N3-C4-C5	-10.91	119.16	126.80
22	BA	502	A	N3-C4-C5	-10.91	119.17	126.80
1	AA	1430	A	C5-C6-N6	10.90	132.42	123.70
1	AA	815	A	C5-C6-N6	10.90	132.42	123.70
22	BA	340	A	C5-C6-N6	10.90	132.42	123.70
22	BA	892	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	2860	A	C5-C6-N6	10.90	132.42	123.70
22	BA	460	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	753	A	N3-C4-C5	-10.90	119.17	126.80
22	BA	819	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	574	A	C5-C6-N6	10.90	132.42	123.70
22	BA	1739	A	N3-C4-C5	-10.90	119.17	126.80
1	AA	1437	A	C5-C6-N6	10.89	132.41	123.70
22	BA	278	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	2741	A	C5-C6-N6	10.89	132.42	123.70
22	BA	346	A	C5-C6-N6	10.89	132.41	123.70
22	BA	382	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	1805	A	C5-C6-N6	10.89	132.41	123.70
1	AA	313	A	C5-C6-N6	10.89	132.41	123.70
22	BA	1373	A	N7-C8-N9	-10.89	108.35	113.80
1	AA	66	A	N7-C8-N9	-10.89	108.36	113.80
1	AA	288	A	C5-C6-N6	10.89	132.41	123.70
1	AA	1492	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	2749	A	C5-C6-N6	10.89	132.41	123.70
22	BA	626	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	2813	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	1366	A	N7-C8-N9	-10.89	108.36	113.80
1	AA	68	G	C4-C5-C6	10.88	125.33	118.80
1	AA	253	A	C5-C6-N6	10.88	132.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	896	A	C5-C6-N6	10.89	132.41	123.70
1	AA	336	A	C5-C6-N6	10.88	132.41	123.70
1	AA	151	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1794	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	2478	A	C5-C6-N6	10.88	132.40	123.70
22	BA	428	A	C5-C6-N6	10.88	132.40	123.70
22	BA	1900	A	C5-C6-N6	10.88	132.40	123.70
22	BA	1938	A	N3-C4-C5	-10.88	119.19	126.80
22	BA	347	A	C5-C6-N6	10.87	132.40	123.70
22	BA	2675	A	N3-C4-C5	-10.87	119.19	126.80
1	AA	622	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	255	A	N7-C8-N9	-10.87	108.37	113.80
22	BA	1679	A	C5-C6-N6	10.87	132.40	123.70
22	BA	265	A	C5-C6-N6	10.87	132.39	123.70
22	BA	1890	A	N7-C8-N9	-10.87	108.37	113.80
1	AA	172	A	C5-C6-N6	10.87	132.39	123.70
1	AA	695	A	C5-C6-N6	10.87	132.39	123.70
22	BA	347	A	N7-C8-N9	-10.87	108.37	113.80
22	BA	2336	A	N7-C8-N9	-10.87	108.37	113.80
1	AA	938	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	2183	A	N7-C8-N9	-10.86	108.37	113.80
1	AA	923	A	N3-C4-C5	-10.86	119.20	126.80
22	BA	1698	A	C5-C6-N6	10.86	132.38	123.70
22	BA	44	A	C5-C6-N6	10.86	132.38	123.70
22	BA	1403	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	2657	A	C5-C6-N6	10.85	132.38	123.70
55	B8	26	A	N7-C8-N9	-10.85	108.37	113.80
1	AA	1346	A	C5-C6-N6	10.85	132.38	123.70
22	BA	750	A	C5-C6-N6	10.85	132.38	123.70
22	BA	877	A	N3-C4-C5	-10.85	119.21	126.80
22	BA	2425	A	C5-C6-N6	10.85	132.38	123.70
54	B7	9	A	N7-C8-N9	-10.85	108.38	113.80
1	AA	1191	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	532	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	222	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2005	A	N7-C8-N9	-10.84	108.38	113.80
1	AA	716	A	C5-C6-N6	10.84	132.37	123.70
22	BA	1789	A	N3-C4-C5	-10.84	119.21	126.80
1	AA	65	A	C5-C6-N6	10.84	132.37	123.70
1	AA	1093	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	384	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	727	A	N7-C8-N9	-10.84	108.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	161	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	1070	A	C5-C6-N6	10.83	132.36	123.70
1	AA	1531	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	896	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1269	A	N7-C8-N9	-10.82	108.39	113.80
1	AA	366	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1829	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1913	A	N7-C8-N9	-10.82	108.39	113.80
1	AA	408	A	C5-C6-N6	10.82	132.36	123.70
1	AA	465	A	N3-C4-C5	-10.82	119.22	126.80
22	BA	2560	A	N3-C4-C5	-10.82	119.22	126.80
1	AA	162	A	N7-C8-N9	-10.82	108.39	113.80
1	AA	1080	A	N7-C8-N9	-10.82	108.39	113.80
1	AA	673	A	N3-C4-C5	-10.82	119.23	126.80
22	BA	251	A	N3-C4-C5	-10.82	119.23	126.80
22	BA	1096	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1241	A	N3-C4-C5	-10.82	119.23	126.80
1	AA	1093	A	C5-C6-N6	10.81	132.35	123.70
23	BB	58	A	N3-C4-C5	-10.81	119.23	126.80
1	AA	983	A	N3-C4-C5	-10.81	119.23	126.80
1	AA	1329	A	C5-C6-N6	10.81	132.35	123.70
22	BA	233	A	C5-C6-N6	10.81	132.35	123.70
22	BA	1413	A	N7-C8-N9	-10.81	108.39	113.80
23	BB	58	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	665	A	C5-C6-N6	10.81	132.35	123.70
55	B8	59	A	N7-C8-N9	-10.81	108.40	113.80
22	BA	103	A	C5-C6-N6	10.81	132.34	123.70
1	AA	865	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	1377	A	C5-C6-N6	10.80	132.34	123.70
3	AC	107	ARG	NE-CZ-NH2	10.80	125.70	120.30
22	BA	2476	A	N7-C8-N9	-10.81	108.40	113.80
22	BA	182	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	1700	A	C5-C6-N6	10.80	132.34	123.70
22	BA	2725	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	1	A	C5-C6-N6	10.80	132.34	123.70
1	AA	448	A	C5-C6-N6	10.80	132.34	123.70
22	BA	56	A	C5-C6-N6	10.80	132.34	123.70
22	BA	64	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	155	A	N3-C4-C5	-10.80	119.24	126.80
1	AA	382	A	C5-C6-N6	10.80	132.34	123.70
1	AA	383	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1872	A	N7-C8-N9	-10.80	108.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	761	A	N3-C4-C5	-10.79	119.24	126.80
22	BA	1780	A	N3-C4-C5	-10.79	119.24	126.80
1	AA	676	A	C5-C6-N6	10.79	132.34	123.70
1	AA	937	A	C5-C6-N6	10.79	132.33	123.70
22	BA	278	A	N3-C4-C5	-10.79	119.25	126.80
22	BA	2376	A	C5-C6-N6	10.79	132.33	123.70
22	BA	2835	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	1090	A	N3-C4-C5	-10.79	119.25	126.80
1	AA	640	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2564	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2577	A	N3-C4-C5	-10.79	119.25	126.80
1	AA	1318	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	2809	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	1509	A	C5-C6-N6	10.78	132.32	123.70
22	BA	2009	A	C5-C6-N6	10.78	132.32	123.70
1	AA	282	A	C5-C6-N6	10.78	132.32	123.70
22	BA	1566	A	C5-C6-N6	10.78	132.32	123.70
22	BA	1237	A	N7-C8-N9	-10.77	108.41	113.80
1	AA	958	A	N7-C8-N9	-10.77	108.41	113.80
1	AA	1507	A	N7-C8-N9	-10.77	108.41	113.80
22	BA	1809	A	N3-C4-C5	-10.77	119.26	126.80
22	BA	149	A	C5-C6-N6	10.77	132.31	123.70
1	AA	510	A	C5-C6-N6	10.77	132.31	123.70
1	AA	1340	A	C5-C6-N6	10.77	132.31	123.70
22	BA	71	A	C5-C6-N6	10.77	132.31	123.70
22	BA	508	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	2868	A	C5-C6-N6	10.77	132.31	123.70
1	AA	98	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	1787	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	2434	A	C5-C6-N6	10.76	132.31	123.70
1	AA	336	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	219	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	1787	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	1669	A	N3-C4-C5	-10.76	119.27	126.80
1	AA	1410	A	C5-C6-N6	10.76	132.30	123.70
1	AA	1238	A	C5-C6-N6	10.75	132.30	123.70
22	BA	127	A	C5-C6-N6	10.75	132.30	123.70
1	AA	865	A	C5-C6-N6	10.75	132.30	123.70
22	BA	146	A	N3-C4-C5	-10.75	119.27	126.80
22	BA	2158	A	N3-C4-C5	-10.75	119.27	126.80
22	BA	2726	A	C5-C6-N6	10.75	132.30	123.70
22	BA	2765	A	N3-C4-C5	-10.75	119.27	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2778	A	N3-C4-C5	-10.75	119.28	126.80
22	BA	1327	A	N7-C8-N9	-10.75	108.43	113.80
22	BA	2461	A	N3-C4-C5	-10.75	119.28	126.80
22	BA	878	A	C5-C6-N6	10.75	132.30	123.70
22	BA	2205	A	N3-C4-C5	-10.75	119.28	126.80
1	AA	1357	A	C5-C6-N6	10.74	132.29	123.70
22	BA	104	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	766	A	C5-C6-N6	10.74	132.29	123.70
22	BA	2097	A	N3-C4-C5	-10.74	119.28	126.80
22	BA	2478	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2792	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2191	A	N3-C4-C5	-10.74	119.28	126.80
55	B8	6	A	C5-C6-N6	10.74	132.29	123.70
1	AA	1363	A	C5-C6-N6	10.73	132.29	123.70
1	AA	77	A	C5-C6-N6	10.73	132.29	123.70
22	BA	590	A	N7-C8-N9	-10.73	108.43	113.80
22	BA	2432	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	80	A	N7-C8-N9	-10.73	108.43	113.80
22	BA	508	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	819	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	1439	A	C5-C6-N6	10.73	132.28	123.70
22	BA	1272	A	C5-C6-N6	10.73	132.28	123.70
22	BA	2284	A	N7-C8-N9	-10.73	108.44	113.80
1	AA	790	A	N7-C8-N9	-10.73	108.44	113.80
55	B8	51	A	C5-C6-N6	10.73	132.28	123.70
22	BA	1365	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2590	A	C5-C6-N6	10.72	132.28	123.70
1	AA	171	A	C5-C6-N6	10.72	132.28	123.70
1	AA	1227	A	C5-C6-N6	10.72	132.28	123.70
22	BA	1773	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	1786	A	N3-C4-C5	-10.72	119.29	126.80
22	BA	1981	A	C5-C6-N6	10.72	132.28	123.70
22	BA	1054	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	2019	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	432	A	C5-C6-N6	10.72	132.27	123.70
22	BA	2377	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	1110	A	C5-C6-N6	10.72	132.27	123.70
1	AA	143	A	C5-C6-N6	10.71	132.27	123.70
1	AA	681	A	C5-C6-N6	10.71	132.27	123.70
22	BA	19	A	N3-C4-C5	-10.71	119.30	126.80
22	BA	412	A	N3-C4-C5	-10.71	119.30	126.80
22	BA	1598	A	N7-C8-N9	-10.71	108.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1847	A	N7-C8-N9	-10.71	108.44	113.80
1	AA	499	A	N3-C4-C5	-10.71	119.30	126.80
22	BA	299	A	N3-C4-C5	-10.71	119.31	126.80
1	AA	51	A	C5-C6-N6	10.71	132.26	123.70
1	AA	559	A	C5-C6-N6	10.71	132.26	123.70
22	BA	95	A	C5-C6-N6	10.70	132.26	123.70
1	AA	1216	A	C5-C6-N6	10.70	132.26	123.70
22	BA	330	A	C5-C6-N6	10.70	132.26	123.70
22	BA	749	A	C5-C6-N6	10.70	132.26	123.70
22	BA	1801	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	2154	A	C5-C6-N6	10.70	132.26	123.70
22	BA	2388	A	N3-C4-C5	-10.70	119.31	126.80
1	AA	1413	A	C5-C6-N6	10.70	132.26	123.70
22	BA	547	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	693	A	N3-C4-C5	-10.69	119.31	126.80
22	BA	928	A	C5-C6-N6	10.69	132.25	123.70
22	BA	1274	A	C5-C6-N6	10.69	132.25	123.70
1	AA	460	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	1039	A	C5-C6-N6	10.69	132.25	123.70
22	BA	1635	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	1735	A	N3-C4-C5	-10.69	119.31	126.80
22	BA	2700	A	N7-C8-N9	-10.69	108.45	113.80
1	AA	1363	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	52	A	C5-C6-N6	10.69	132.25	123.70
22	BA	429	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	1151	A	N3-C4-C5	-10.69	119.32	126.80
22	BA	1632	A	C5-C6-N6	10.69	132.25	123.70
1	AA	50	A	C5-C6-N6	10.68	132.25	123.70
22	BA	1783	A	C5-N7-C8	10.68	109.24	103.90
22	BA	2459	A	N3-C4-C5	-10.68	119.32	126.80
1	AA	374	A	N3-C4-C5	-10.68	119.32	126.80
55	B8	76	A	N9-C4-C5	10.68	110.07	105.80
1	AA	825	A	C5-C6-N6	10.68	132.24	123.70
22	BA	1872	A	N3-C4-C5	-10.68	119.32	126.80
1	AA	1005	A	N3-C4-C5	-10.68	119.33	126.80
22	BA	1284	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	2764	A	N3-C4-C5	-10.68	119.33	126.80
1	AA	560	A	N7-C8-N9	-10.67	108.46	113.80
22	BA	2015	A	N7-C8-N9	-10.67	108.46	113.80
1	AA	923	A	N7-C8-N9	-10.67	108.46	113.80
1	AA	1082	A	N7-C8-N9	-10.67	108.47	113.80
22	BA	2031	A	C5-C6-N6	10.67	132.24	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2547	A	C5-C6-N6	10.67	132.24	123.70
22	BA	2887	A	C5-C6-N6	10.67	132.24	123.70
1	AA	996	A	C5-C6-N6	10.67	132.23	123.70
22	BA	845	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	2278	A	N7-C8-N9	-10.67	108.47	113.80
1	AA	767	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	780	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	1261	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1274	A	N3-C4-C5	-10.66	119.34	126.80
22	BA	1230	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	1394	A	C5-C6-N6	10.66	132.23	123.70
1	AA	1398	A	C5-C6-N6	10.66	132.23	123.70
22	BA	655	A	C5-C6-N6	10.66	132.22	123.70
22	BA	1304	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	2114	A	C5-C6-N6	10.66	132.23	123.70
1	AA	389	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	1205	A	C5-C6-N6	10.65	132.22	123.70
1	AA	223	A	N7-C8-N9	-10.65	108.47	113.80
22	BA	241	A	C5-C6-N6	10.65	132.22	123.70
22	BA	526	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	2411	A	C5-C6-N6	10.65	132.22	123.70
22	BA	592	A	C5-C6-N6	10.65	132.22	123.70
22	BA	705	A	N7-C8-N9	-10.65	108.48	113.80
22	BA	753	A	C5-C6-N6	10.64	132.22	123.70
22	BA	1001	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	1269	A	C5-C6-N6	10.64	132.22	123.70
22	BA	2823	A	N3-C4-C5	-10.64	119.35	126.80
1	AA	935	A	C5-C6-N6	10.64	132.21	123.70
22	BA	1528	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1932	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	2090	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	2135	A	N3-C4-C5	-10.64	119.35	126.80
55	B8	26	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1353	A	C5-C6-N6	10.64	132.21	123.70
1	AA	1507	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	2700	A	C5-C6-N6	10.64	132.21	123.70
1	AA	1508	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	94	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1321	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	781	A	C5-C6-N6	10.63	132.20	123.70
22	BA	2425	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	2887	A	N7-C8-N9	-10.63	108.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1280	A	C5-C6-N6	10.63	132.20	123.70
1	AA	320	A	C5-C6-N6	10.63	132.20	123.70
22	BA	2003	A	C5-C6-N6	10.63	132.20	123.70
22	BA	574	A	C5-C6-N6	10.63	132.20	123.70
1	AA	1350	A	C5-C6-N6	10.62	132.20	123.70
1	AA	1368	A	C5-C6-N6	10.62	132.20	123.70
22	BA	2336	A	C5-C6-N6	10.63	132.20	123.70
22	BA	1268	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	2598	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	792	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	160	A	C5-C6-N6	10.62	132.20	123.70
1	AA	977	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	352	A	C5-C6-N6	10.62	132.19	123.70
55	B8	59	A	C5-C6-N6	10.62	132.19	123.70
22	BA	480	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	1214	A	C5-C6-N6	10.61	132.19	123.70
22	BA	2184	A	N7-C8-N9	-10.61	108.49	113.80
22	BA	522	A	N7-C8-N9	-10.61	108.50	113.80
1	AA	181	A	C5-C6-N6	10.61	132.18	123.70
1	AA	415	A	N7-C8-N9	-10.61	108.50	113.80
1	AA	559	A	N3-C4-C5	-10.61	119.38	126.80
22	BA	449	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	2059	A	N3-C4-C5	-10.60	119.38	126.80
23	BB	57	A	N7-C8-N9	-10.60	108.50	113.80
1	AA	728	A	C5-C6-N6	10.60	132.18	123.70
22	BA	454	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	472	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	1901	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	2147	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1603	A	N7-C8-N9	-10.60	108.50	113.80
1	AA	55	A	C5-C6-N6	10.60	132.18	123.70
1	AA	746	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	190	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	2333	A	C5-C6-N6	10.60	132.18	123.70
1	AA	1275	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1890	A	C5-C6-N6	10.60	132.18	123.70
22	BA	2679	A	N7-C8-N9	-10.60	108.50	113.80
1	AA	621	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	449	A	C5-C6-N6	10.59	132.17	123.70
1	AA	819	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1336	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	2516	A	C5-C6-N6	10.59	132.17	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	19	A	N7-C8-N9	-10.59	108.51	113.80
1	AA	1271	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1367	A	C5-C6-N6	10.59	132.17	123.70
22	BA	2015	A	C5-C6-N6	10.59	132.17	123.70
22	BA	2205	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1050	A	C5-C6-N6	10.58	132.17	123.70
22	BA	125	A	C5-C6-N6	10.58	132.16	123.70
1	AA	949	A	N3-C4-C5	-10.58	119.39	126.80
1	AA	495	A	C5-C6-N6	10.58	132.16	123.70
1	AA	655	A	N3-C4-C5	-10.58	119.40	126.80
22	BA	2054	A	N3-C4-C5	-10.58	119.39	126.80
1	AA	1130	A	N7-C8-N9	-10.58	108.51	113.80
22	BA	2170	A	C5-C6-N6	10.58	132.16	123.70
22	BA	83	A	C5-C6-N6	10.57	132.16	123.70
22	BA	706	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	1987	A	C5-C6-N6	10.57	132.16	123.70
1	AA	718	A	N7-C8-N9	-10.57	108.51	113.80
1	AA	889	A	N7-C8-N9	-10.57	108.51	113.80
22	BA	1057	A	N7-C8-N9	-10.57	108.51	113.80
22	BA	1419	A	C5-C6-N6	10.57	132.16	123.70
22	BA	2328	A	N7-C8-N9	-10.57	108.51	113.80
1	AA	716	A	N3-C4-C5	-10.57	119.40	126.80
1	AA	199	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	161	A	C5-C6-N6	10.57	132.15	123.70
22	BA	1590	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	1677	A	C5-C6-N6	10.57	132.15	123.70
1	AA	1225	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	204	A	C5-C6-N6	10.56	132.15	123.70
22	BA	616	A	C5-C6-N6	10.56	132.15	123.70
22	BA	631	A	C5-C6-N6	10.56	132.15	123.70
22	BA	807	U	C2-N3-C4	-10.56	120.66	127.00
22	BA	632	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	1809	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	1050	A	N3-C4-C5	-10.56	119.41	126.80
1	AA	978	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	1433	A	C5-C6-N6	10.56	132.15	123.70
22	BA	1591	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	2114	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	2274	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	1456	A	C5-C6-N6	10.55	132.14	123.70
22	BA	752	A	C5-N7-C8	10.55	109.17	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1000	A	N7-C8-N9	-10.55	108.53	113.80
1	AA	675	A	C5-C6-N6	10.55	132.14	123.70
1	AA	151	A	N3-C4-C5	-10.55	119.42	126.80
22	BA	2560	A	N7-C8-N9	-10.55	108.53	113.80
1	AA	60	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	451	A	C5-C6-N6	10.55	132.14	123.70
22	BA	1439	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	53	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	502	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	1171	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	80	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	492	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	782	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	1746	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	1819	A	C5-C6-N6	10.53	132.13	123.70
22	BA	1889	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	696	A	C5-C6-N6	10.53	132.12	123.70
22	BA	300	A	N7-C8-N9	-10.53	108.54	113.80
22	BA	1668	A	N3-C4-C5	-10.53	119.43	126.80
22	BA	2070	A	N3-C4-C5	-10.53	119.43	126.80
22	BA	1230	A	C5-C6-N6	10.53	132.12	123.70
1	AA	26	A	C5-C6-N6	10.52	132.12	123.70
1	AA	174	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	415	A	C5-C6-N6	10.52	132.12	123.70
22	BA	504	A	N3-C4-C5	-10.52	119.43	126.80
22	BA	1014	A	C5-C6-N6	10.52	132.12	123.70
22	BA	2198	A	C5-C6-N6	10.52	132.12	123.70
1	AA	374	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	1229	A	C5-C6-N6	10.52	132.11	123.70
22	BA	2654	A	C5-C6-N6	10.52	132.12	123.70
1	AA	397	A	C5-C6-N6	10.52	132.11	123.70
1	AA	642	A	C5-C6-N6	10.52	132.11	123.70
22	BA	362	A	N3-C4-C5	-10.52	119.44	126.80
22	BA	2328	A	N3-C4-C5	-10.52	119.44	126.80
1	AA	1250	A	C5-C6-N6	10.51	132.11	123.70
1	AA	702	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	172	A	C5-C6-N6	10.51	132.11	123.70
22	BA	2761	A	N3-C4-C5	-10.51	119.44	126.80
1	AA	205	A	C5-C6-N6	10.51	132.10	123.70
1	AA	431	A	N7-C8-N9	-10.50	108.55	113.80
1	AA	807	A	N7-C8-N9	-10.50	108.55	113.80
1	AA	630	A	C5-C6-N6	10.50	132.10	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	108	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1189	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	2191	A	C5-C6-N6	10.50	132.10	123.70
1	AA	784	A	N3-C4-C5	-10.49	119.45	126.80
22	BA	1998	A	N3-C4-C5	-10.49	119.45	126.80
1	AA	303	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1085	A	N3-C4-C5	-10.49	119.45	126.80
22	BA	1354	A	N3-C4-C5	-10.49	119.46	126.80
1	AA	236	A	C5-C6-N6	10.49	132.09	123.70
1	AA	959	A	C5-C6-N6	10.49	132.09	123.70
1	AA	1014	A	C5-C6-N6	10.49	132.09	123.70
1	AA	649	A	C5-C6-N6	10.49	132.09	123.70
1	AA	1152	A	N3-C4-C5	-10.49	119.46	126.80
22	BA	309	A	N3-C4-C5	-10.48	119.46	126.80
22	BA	1970	A	N3-C4-C5	-10.48	119.46	126.80
1	AA	782	A	N7-C8-N9	-10.48	108.56	113.80
1	AA	1394	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	1998	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	2662	A	C5-C6-N6	10.48	132.08	123.70
1	AA	383	A	N3-C4-C5	-10.48	119.47	126.80
22	BA	574	A	N3-C4-C5	-10.48	119.47	126.80
1	AA	1229	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	984	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	1901	A	N7-C8-N9	-10.48	108.56	113.80
55	B8	66	A	C5-C6-N6	10.48	132.08	123.70
1	AA	1492	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	2426	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	1583	A	C5-C6-N6	10.47	132.08	123.70
1	AA	300	A	C4-C5-C6	10.47	122.23	117.00
22	BA	1952	A	C5-C6-N6	10.47	132.08	123.70
22	BA	1791	A	N7-C8-N9	-10.47	108.57	113.80
22	BA	1848	A	N3-C4-C5	-10.47	119.47	126.80
1	AA	968	A	C5-C6-N6	10.46	132.07	123.70
22	BA	614	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1810	A	C4-C5-C6	10.46	122.23	117.00
22	BA	2377	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	2614	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	792	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1126	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	1396	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	2829	A	C5-N7-C8	10.46	109.13	103.90
1	AA	327	A	C5-C6-N6	10.46	132.07	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	217	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	294	A	C5-C6-N6	10.46	132.07	123.70
23	BB	15	A	C5-C6-N6	10.46	132.06	123.70
1	AA	1236	A	N3-C4-C5	-10.45	119.48	126.80
1	AA	356	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	1496	A	N7-C8-N9	-10.45	108.57	113.80
22	BA	1654	A	N7-C8-N9	-10.45	108.57	113.80
22	BA	2009	A	N7-C8-N9	-10.45	108.58	113.80
22	BA	2014	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	116	A	OP2-P-O3'	-10.45	82.21	105.20
22	BA	391	A	N3-C4-C5	-10.45	119.48	126.80
55	B8	58	A	C5-C6-N6	10.45	132.06	123.70
22	BA	2142	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	743	A	N3-C4-C5	-10.45	119.49	126.80
23	BB	53	A	C5-C6-N6	10.45	132.06	123.70
22	BA	911	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	1366	A	C5-C6-N6	10.44	132.05	123.70
1	AA	553	A	C5-C6-N6	10.44	132.05	123.70
1	AA	69	G	O4'-C1'-N9	10.44	116.55	108.20
1	AA	466	A	N7-C8-N9	-10.44	108.58	113.80
1	AA	1441	A	C5-C6-N6	10.44	132.05	123.70
1	AA	831	A	C5-C6-N6	10.44	132.05	123.70
1	AA	635	A	C5-C6-N6	10.44	132.05	123.70
22	BA	532	A	N3-C4-C5	-10.44	119.50	126.80
22	BA	1287	A	N3-C4-C5	-10.44	119.50	126.80
22	BA	1095	A	N3-C4-C5	-10.43	119.50	126.80
1	AA	78	A	C5-C6-N6	10.43	132.04	123.70
22	BA	322	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	2675	A	C5-C6-N6	10.43	132.04	123.70
22	BA	382	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1276	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1544	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	2388	A	C5-N7-C8	10.43	109.11	103.90
1	AA	279	A	C5-C6-N6	10.42	132.04	123.70
1	AA	321	A	N3-C4-C5	-10.42	119.51	126.80
22	BA	2378	A	N7-C8-N9	-10.42	108.59	113.80
1	AA	509	A	C5-C6-N6	10.42	132.03	123.70
22	BA	909	A	N7-C8-N9	-10.42	108.59	113.80
1	AA	192	A	N3-C4-C5	-10.42	119.51	126.80
22	BA	300	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	781	A	C5-C6-N6	10.41	132.03	123.70
22	BA	278	A	C5-C6-N6	10.41	132.03	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	66	A	N7-C8-N9	-10.41	108.59	113.80
1	AA	1261	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	1306	A	C5-C6-N6	10.41	132.03	123.70
22	BA	1494	A	N7-C8-N9	-10.41	108.59	113.80
1	AA	139	A	N3-C4-C5	-10.41	119.52	126.80
1	AA	1246	A	N3-C4-C5	-10.41	119.52	126.80
22	BA	49	A	C5-C6-N6	10.41	132.03	123.70
22	BA	101	A	N7-C8-N9	-10.41	108.60	113.80
22	BA	2634	A	C5-C6-N6	10.41	132.03	123.70
22	BA	2813	A	N3-C4-C5	-10.40	119.52	126.80
1	AA	3	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	28	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1477	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1749	A	C5-C6-N6	10.40	132.02	123.70
22	BA	217	A	C5-C6-N6	10.40	132.02	123.70
22	BA	2893	A	C5-C6-N6	10.40	132.02	123.70
22	BA	2352	A	N7-C8-N9	-10.40	108.60	113.80
1	AA	747	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2407	A	N3-C4-C5	-10.40	119.52	126.80
1	AA	1418	A	N7-C8-N9	-10.39	108.60	113.80
22	BA	892	A	N3-C4-C5	-10.39	119.52	126.80
22	BA	2497	A	C5-C6-N6	10.39	132.02	123.70
1	AA	1375	A	C5-C6-N6	10.39	132.01	123.70
1	AA	1493	A	C5-C6-N6	10.39	132.01	123.70
22	BA	1151	A	C5-C6-N6	10.39	132.01	123.70
22	BA	1307	A	N7-C8-N9	-10.39	108.60	113.80
1	AA	1408	A	C5-C6-N6	10.39	132.01	123.70
22	BA	470	A	N3-C4-C5	-10.39	119.53	126.80
22	BA	1801	A	C5-C6-N6	10.39	132.01	123.70
22	BA	2327	A	N3-C4-C5	-10.39	119.53	126.80
22	BA	38	A	N3-C4-C5	-10.38	119.53	126.80
22	BA	2826	A	C5-C6-N6	10.38	132.01	123.70
1	AA	338	A	N3-C4-C5	-10.38	119.53	126.80
23	BB	53	A	N3-C4-C5	-10.38	119.53	126.80
22	BA	1413	A	C5-C6-N6	10.38	132.00	123.70
1	AA	267	C	O5'-P-OP2	-10.38	96.36	105.70
22	BA	2635	A	N3-C4-C5	-10.38	119.54	126.80
1	AA	974	A	C5-C6-N6	10.37	132.00	123.70
1	AA	1012	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	244	A	N7-C8-N9	-10.37	108.61	113.80
22	BA	1226	A	N3-C4-C5	-10.37	119.54	126.80
1	AA	909	A	N7-C8-N9	-10.37	108.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	538	A	C5-C6-N6	10.37	132.00	123.70
22	BA	1069	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	1086	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	2288	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	2740	A	C5-C6-N6	10.37	132.00	123.70
22	BA	347	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	2635	A	N7-C8-N9	-10.37	108.62	113.80
1	AA	1005	A	N7-C8-N9	-10.37	108.62	113.80
22	BA	2080	A	C5-C6-N6	10.37	131.99	123.70
22	BA	2531	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	2736	A	C5-C6-N6	10.37	131.99	123.70
1	AA	1196	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2077	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	768	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	162	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	1238	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	959	A	C5-C6-N6	10.36	131.99	123.70
1	AA	900	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	547	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	1744	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	600	A	C5-C6-N6	10.35	131.98	123.70
22	BA	575	A	C5-C6-N6	10.35	131.98	123.70
22	BA	2766	A	C5-C6-N6	10.35	131.98	123.70
1	AA	959	A	N3-C4-C5	-10.35	119.56	126.80
22	BA	460	A	C5-C6-N6	10.35	131.98	123.70
22	BA	633	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	1009	A	C8-N9-C4	10.35	109.94	105.80
22	BA	2792	A	N3-C4-C5	-10.35	119.56	126.80
1	AA	131	A	C5-C6-N6	10.35	131.98	123.70
22	BA	2101	A	N3-C4-C5	-10.35	119.56	126.80
22	BA	877	A	C5-C6-N6	10.34	131.97	123.70
22	BA	176	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	752	A	C4-C5-N7	-10.34	105.53	110.70
22	BA	1268	A	C5-C6-N6	10.34	131.97	123.70
22	BA	13	A	C5-C6-N6	10.34	131.97	123.70
22	BA	685	A	C5-C6-N6	10.34	131.97	123.70
55	B8	41	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	627	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	196	A	C5-C6-N6	10.34	131.97	123.70
1	AA	228	A	C5-C6-N6	10.34	131.97	123.70
22	BA	142	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	861	A	C5-C6-N6	10.34	131.97	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	913	A	C5-C6-N6	10.34	131.97	123.70
22	BA	1373	A	N3-C4-C5	-10.34	119.57	126.80
1	AA	539	A	N3-C4-C5	-10.33	119.57	126.80
1	AA	629	A	C5-C6-N6	10.33	131.97	123.70
1	AA	1082	A	C5-C6-N6	10.33	131.97	123.70
22	BA	513	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	2639	A	C5-C6-N6	10.33	131.97	123.70
22	BA	984	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	1744	A	N7-C8-N9	-10.33	108.63	113.80
22	BA	478	A	C5-C6-N6	10.33	131.96	123.70
22	BA	1597	A	C5-C6-N6	10.33	131.96	123.70
23	BB	101	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	56	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	2268	A	C5-C6-N6	10.33	131.96	123.70
1	AA	452	A	C5-C6-N6	10.32	131.96	123.70
22	BA	2837	A	C5-C6-N6	10.32	131.96	123.70
22	BA	471	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	789	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	1082	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	1483	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	382	A	C5-C6-N6	10.32	131.96	123.70
1	AA	845	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	1226	A	C5-C6-N6	10.32	131.95	123.70
23	BB	101	A	C5-C6-N1	10.32	122.86	117.70
1	AA	1157	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	156	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	1927	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	2088	A	C5-C6-N6	10.31	131.95	123.70
22	BA	2117	A	C5-C6-N6	10.31	131.95	123.70
22	BA	2281	A	C5-C6-N6	10.31	131.95	123.70
22	BA	2766	A	N3-C4-C5	-10.31	119.58	126.80
1	AA	430	A	N3-C4-C5	-10.31	119.58	126.80
1	AA	1357	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	1103	A	C5-C6-N6	10.31	131.95	123.70
22	BA	1549	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	1579	A	C5-C6-N6	10.31	131.95	123.70
1	AA	780	A	N3-C4-C5	-10.31	119.59	126.80
1	AA	509	A	N3-C4-C5	-10.30	119.59	126.80
1	AA	728	A	N3-C4-C5	-10.30	119.59	126.80
1	AA	949	A	C5-C6-N6	10.30	131.94	123.70
23	BB	46	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	1889	A	C5-C6-N6	10.30	131.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2247	A	C5-C6-N6	10.30	131.94	123.70
22	BA	2459	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	1077	A	C5-C6-N6	10.30	131.94	123.70
22	BA	1571	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	2412	A	C5-C6-N6	10.30	131.94	123.70
1	AA	1311	A	N3-C4-C5	-10.30	119.59	126.80
1	AA	716	A	N7-C8-N9	-10.29	108.65	113.80
22	BA	900	A	C5-C6-N6	10.29	131.94	123.70
22	BA	2565	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	515	A	C5-C6-N6	10.29	131.93	123.70
1	AA	499	A	C5-C6-N6	10.28	131.93	123.70
22	BA	706	A	C5-C6-N6	10.29	131.93	123.70
22	BA	1254	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	1275	A	C5-C6-N6	10.29	131.93	123.70
1	AA	116	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	219	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	705	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1156	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	197	A	C5-C6-N6	10.28	131.93	123.70
22	BA	1490	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	2706	A	N3-C4-C5	-10.28	119.60	126.80
1	AA	1046	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	705	A	C5-C6-N6	10.28	131.92	123.70
22	BA	990	A	C5-C6-N6	10.28	131.92	123.70
1	AA	900	A	N3-C4-C5	-10.28	119.61	126.80
1	AA	1150	A	C5-C6-N6	10.28	131.92	123.70
22	BA	609	A	C5-C6-N6	10.28	131.92	123.70
22	BA	793	A	N3-C4-C5	-10.28	119.61	126.80
1	AA	1318	A	C5-C6-N6	10.27	131.92	123.70
22	BA	1403	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	1339	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	1080	A	C5-C6-N6	10.27	131.92	123.70
22	BA	1241	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	1705	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	459	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	873	A	C5-C6-N6	10.27	131.91	123.70
1	AA	1225	A	C5-C6-N6	10.26	131.91	123.70
22	BA	1586	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	2015	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	298	A	C5-C6-N6	10.26	131.91	123.70
22	BA	1571	A	C5-C6-N6	10.26	131.91	123.70
22	BA	2082	A	C5-C6-N6	10.26	131.91	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1420	A	C5-C6-N6	10.26	131.91	123.70
22	BA	1746	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	2614	A	C5-N7-C8	10.26	109.03	103.90
1	AA	802	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	1021	A	C5-C6-N6	10.25	131.90	123.70
1	AA	1375	A	N3-C4-C5	-10.25	119.62	126.80
23	BB	46	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	2020	A	C5-C6-N6	10.25	131.90	123.70
1	AA	1274	A	C5-C6-N6	10.25	131.90	123.70
22	BA	95	A	N7-C8-N9	-10.25	108.67	113.80
22	BA	849	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	1786	A	N7-C8-N9	-10.25	108.67	113.80
22	BA	2388	A	C5-C6-N6	10.25	131.90	123.70
22	BA	14	A	N7-C8-N9	-10.25	108.68	113.80
22	BA	221	A	C5-C6-N6	10.25	131.90	123.70
22	BA	2809	A	C5-C6-N6	10.25	131.90	123.70
1	AA	3	A	C5-C6-N6	10.24	131.90	123.70
22	BA	1080	A	N7-C8-N9	-10.24	108.68	113.80
1	AA	663	A	C5-C6-N6	10.24	131.90	123.70
22	BA	1535	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	2340	A	C8-N9-C4	10.24	109.90	105.80
22	BA	2705	A	C5-C6-N6	10.24	131.89	123.70
1	AA	596	A	C5-C6-N6	10.24	131.89	123.70
22	BA	1244	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	325	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	373	A	C5-C6-N6	10.24	131.89	123.70
1	AA	493	A	C5-C6-N6	10.24	131.89	123.70
22	BA	1000	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	1535	A	N3-C4-C5	-10.24	119.64	126.80
1	AA	560	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	815	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	2497	A	C4-C5-C6	10.23	122.12	117.00
22	BA	2542	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	1180	A	C5-C6-N6	10.23	131.89	123.70
1	AA	630	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	32	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	44	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	238	A	C5-C6-N6	10.22	131.88	123.70
1	AA	270	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	864	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	906	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	1080	A	C5-C6-N6	10.22	131.88	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	478	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	1347	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	1469	A	C5-C6-N6	10.22	131.88	123.70
22	BA	2199	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	496	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	1308	A	N3-C4-C5	-10.21	119.65	126.80
22	BA	1383	A	N3-C4-C5	-10.21	119.65	126.80
1	AA	1418	A	N3-C4-C5	-10.21	119.65	126.80
1	AA	1476	A	C5-C6-N6	10.21	131.87	123.70
1	AA	167	A	N3-C4-C5	-10.21	119.65	126.80
22	BA	1614	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	1773	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	2335	A	C5-N7-C8	10.21	109.01	103.90
22	BA	2758	A	C5-C6-N6	10.21	131.87	123.70
1	AA	131	A	N3-C4-C5	-10.21	119.66	126.80
1	AA	435	A	C5-C6-N6	10.21	131.87	123.70
22	BA	980	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	1286	A	C5-C6-N6	10.21	131.86	123.70
22	BA	1580	A	C5-C6-N6	10.20	131.86	123.70
1	AA	1500	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	655	A	N3-C4-C5	-10.20	119.66	126.80
55	B8	69	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	1503	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	2721	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	512	G	O4'-C1'-N9	10.20	116.36	108.20
22	BA	627	A	C5-C6-N6	10.20	131.86	123.70
1	AA	33	A	C5-C6-N6	10.19	131.85	123.70
22	BA	899	A	C5-C6-N6	10.20	131.86	123.70
1	AA	1152	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	428	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	1010	A	C5-C6-N6	10.19	131.85	123.70
22	BA	2266	A	C5-C6-N6	10.19	131.85	123.70
1	AA	907	A	N3-C4-C5	-10.19	119.67	126.80
1	AA	1495	U	N1-C2-O2	10.19	129.93	122.80
1	AA	366	A	C5-C6-N6	10.19	131.85	123.70
1	AA	747	A	N7-C8-N9	-10.19	108.70	113.80
1	AA	414	A	C5-C6-N6	10.19	131.85	123.70
22	BA	218	A	C5-C6-N6	10.19	131.85	123.70
1	AA	498	A	C5-C6-N1	10.19	122.79	117.70
22	BA	1090	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	782	A	C5-C6-N6	10.18	131.84	123.70
1	AA	349	A	C5-C6-N6	10.18	131.84	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	241	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	918	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	1913	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	2176	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	50	A	N3-C4-C5	-10.18	119.68	126.80
22	BA	2071	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	523	A	C5-C6-N6	10.17	131.84	123.70
1	AA	975	A	C5-C6-N6	10.17	131.84	123.70
22	BA	101	A	C5-C6-N6	10.17	131.84	123.70
22	BA	344	A	C5-C6-N6	10.17	131.84	123.70
22	BA	2117	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2764	A	N7-C8-N9	-10.17	108.71	113.80
22	BA	582	A	N7-C8-N9	-10.17	108.71	113.80
22	BA	1103	A	N7-C8-N9	-10.17	108.72	113.80
22	BA	1077	A	N7-C8-N9	-10.17	108.72	113.80
22	BA	1885	A	N3-C4-C5	-10.17	119.68	126.80
1	AA	44	A	N3-C4-C5	-10.17	119.68	126.80
1	AA	205	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	306	A	C5-C6-N6	10.16	131.83	123.70
22	BA	167	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	1134	A	C5-C6-N6	10.16	131.83	123.70
1	AA	946	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	1238	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	896	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	2101	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	1219	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	849	A	C5-C6-N6	10.16	131.83	123.70
22	BA	1549	A	C5-C6-N6	10.16	131.83	123.70
1	AA	595	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	1088	A	C5-C6-N6	10.16	131.82	123.70
22	BA	2868	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	547	A	N3-C4-C5	-10.15	119.69	126.80
1	AA	2	A	C5-C6-N6	10.15	131.82	123.70
1	AA	1534	A	C5-C6-N6	10.15	131.82	123.70
22	BA	2314	A	N3-C4-C5	-10.15	119.69	126.80
1	AA	1155	A	C5-C6-N6	10.15	131.82	123.70
22	BA	478	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	1029	A	C5-C6-N6	10.15	131.82	123.70
1	AA	640	A	C5-C6-N6	10.15	131.82	123.70
23	BB	57	A	C5-C6-N6	10.15	131.82	123.70
22	BA	1048	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	1572	A	N3-C4-C5	-10.15	119.70	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2765	A	C5-C6-N6	10.15	131.82	123.70
22	BA	722	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	2738	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	528	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1387	A	C5-C6-N6	10.14	131.81	123.70
1	AA	393	A	C5-C6-N6	10.14	131.81	123.70
22	BA	715	A	C5-C6-N6	10.14	131.81	123.70
22	BA	2082	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	2757	A	C5-C6-N6	10.14	131.81	123.70
22	BA	1515	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	752	A	N7-C8-N9	-10.13	108.73	113.80
22	BA	2814	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	342	A	C5-C6-N6	10.13	131.81	123.70
22	BA	2154	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	1936	A	C5-C6-N6	10.13	131.80	123.70
22	BA	2005	A	N3-C4-C5	-10.13	119.71	126.80
23	BB	108	A	N3-C4-C5	-10.13	119.71	126.80
1	AA	1430	A	N7-C8-N9	-10.13	108.74	113.80
22	BA	2665	A	C5-C6-N6	10.13	131.80	123.70
55	B8	14	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	582	A	C5-C6-N6	10.13	131.80	123.70
22	BA	1111	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	1096	A	N3-C4-C5	-10.12	119.71	126.80
22	BA	104	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	1151	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	583	A	C5-N7-C8	10.12	108.96	103.90
22	BA	911	A	C5-C6-N6	10.12	131.80	123.70
22	BA	2169	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	2513	A	N3-C4-C5	-10.12	119.72	126.80
23	BB	39	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	213	A	C5-C6-N6	10.11	131.79	123.70
22	BA	783	A	N7-C8-N9	-10.11	108.74	113.80
22	BA	480	A	C5-C6-N6	10.11	131.79	123.70
1	AA	199	A	N7-C8-N9	-10.11	108.74	113.80
1	AA	366	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	213	A	C8-N9-C4	10.11	109.84	105.80
22	BA	332	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	693	A	C5-N7-C8	10.11	108.96	103.90
22	BA	2369	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	2736	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	451	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	873	A	N3-C4-C5	-10.11	119.72	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	935	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	504	A	C5-C6-N6	10.11	131.79	123.70
1	AA	704	A	C5-C6-N6	10.11	131.79	123.70
1	AA	478	A	N3-C4-C5	-10.11	119.73	126.80
22	BA	279	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	2434	A	N3-C4-C5	-10.11	119.73	126.80
1	AA	696	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1912	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	2142	A	N7-C8-N9	-10.10	108.75	113.80
55	B8	26	A	C5-C6-N6	10.10	131.78	123.70
1	AA	1055	A	C5-C6-N6	10.10	131.78	123.70
22	BA	1213	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	362	A	C5-C6-N6	10.10	131.78	123.70
55	B8	76	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	981	A	N7-C8-N9	-10.09	108.75	113.80
22	BA	1754	A	C5-C6-N6	10.09	131.77	123.70
1	AA	28	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	454	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	1254	A	C5-C6-N6	10.09	131.77	123.70
22	BA	172	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	905	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	1103	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	1669	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	2814	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	1609	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	1301	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	670	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1789	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	1987	A	C5-N7-C8	10.08	108.94	103.90
22	BA	2577	A	C5-C6-N6	10.08	131.77	123.70
22	BA	1077	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	2211	A	C5-C6-N6	10.08	131.76	123.70
22	BA	471	A	C5-C6-N6	10.08	131.76	123.70
22	BA	751	A	N7-C8-N9	-10.07	108.76	113.80
23	BB	15	A	N7-C8-N9	-10.07	108.76	113.80
22	BA	1780	A	N7-C8-N9	-10.07	108.76	113.80
1	AA	968	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	1219	A	N7-C8-N9	-10.07	108.77	113.80
1	AA	1433	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	497	A	C5-C6-N6	10.07	131.76	123.70
22	BA	644	A	C5-C6-N6	10.07	131.76	123.70
22	BA	1665	A	N3-C4-C5	-10.07	119.75	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2872	A	C5-N7-C8	10.07	108.94	103.90
22	BA	654	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1143	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	2171	A	C5-C6-N6	10.07	131.75	123.70
1	AA	908	A	N3-C4-C5	-10.06	119.75	126.80
1	AA	321	A	C5-C6-N6	10.06	131.75	123.70
1	AA	969	A	C5-C6-N6	10.06	131.75	123.70
22	BA	1609	A	C5-C6-N6	10.06	131.75	123.70
55	B8	59	A	N3-C4-C5	-10.06	119.75	126.80
1	AA	389	A	C5-C6-N6	10.06	131.75	123.70
22	BA	255	A	C5-C6-N6	10.06	131.75	123.70
22	BA	1953	A	C5-C6-N6	10.06	131.75	123.70
22	BA	2031	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	1805	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	2126	A	C5-C6-N6	10.05	131.74	123.70
22	BA	2212	A	N3-C4-C5	-10.05	119.76	126.80
1	AA	1012	A	C5-C6-N6	10.05	131.74	123.70
1	AA	329	A	N3-C4-C5	-10.05	119.76	126.80
22	BA	460	A	N3-C4-C5	-10.05	119.76	126.80
22	BA	2781	A	N7-C8-N9	-10.05	108.78	113.80
1	AA	456	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	1117	A	C5-C6-N6	10.05	131.74	123.70
1	AA	938	A	C5-C6-N6	10.04	131.74	123.70
22	BA	21	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2317	A	C5-C6-N6	10.04	131.73	123.70
22	BA	1169	A	C5-C6-N6	10.04	131.73	123.70
55	B8	41	A	C5-C6-N6	10.04	131.73	123.70
1	AA	573	A	C5-C6-N6	10.04	131.73	123.70
22	BA	2322	A	C5-C6-N6	10.04	131.73	123.70
22	BA	1088	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1679	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	753	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	2639	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1155	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2706	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	2850	A	C5-C6-N6	10.03	131.72	123.70
22	BA	2108	A	N7-C8-N9	-10.03	108.79	113.80
1	AA	1493	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2191	A	N7-C8-N9	-10.02	108.79	113.80
1	AA	364	A	N3-C4-C5	-10.02	119.78	126.80
1	AA	1357	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	374	A	N3-C4-C5	-10.02	119.79	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2850	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1004	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	1008	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	492	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	845	A	C5-C6-N6	10.02	131.71	123.70
22	BA	2003	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	1040	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	2711	A	C5-C6-N6	10.01	131.71	123.70
23	BB	57	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	526	A	C5-N7-C8	10.01	108.91	103.90
22	BA	1073	A	N3-C4-C5	-10.01	119.79	126.80
1	AA	1146	A	C5-C6-N6	10.01	131.71	123.70
22	BA	1008	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	1953	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	152	A	C5-C6-N6	10.00	131.70	123.70
22	BA	1759	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	2435	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	901	A	C4-C5-C6	10.00	122.00	117.00
1	AA	1446	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1350	A	N3-C4-C5	-9.99	119.80	126.80
22	BA	320	A	C5-C6-N6	9.99	131.70	123.70
1	AA	994	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	1349	A	C5-C6-N6	9.99	131.69	123.70
22	BA	1705	A	C5-C6-N6	9.99	131.69	123.70
22	BA	2183	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	829	A	C5-C6-N6	9.99	131.69	123.70
22	BA	2654	A	N7-C8-N9	-9.99	108.81	113.80
22	BA	833	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	1143	A	C5-C6-N6	9.98	131.69	123.70
22	BA	1932	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	632	A	C5-C6-N6	9.98	131.68	123.70
22	BA	1854	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	751	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	2531	A	C5-C6-N6	9.97	131.68	123.70
22	BA	2856	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2534	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	502	A	N7-C8-N9	-9.97	108.82	113.80
22	BA	572	A	C5-C6-N6	9.97	131.67	123.70
22	BA	781	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2080	A	N3-C4-C5	-9.97	119.82	126.80
23	BB	66	A	C5-C6-N6	9.97	131.67	123.70
1	AA	408	A	N3-C4-C5	-9.97	119.82	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	348	A	C5-C6-N6	9.96	131.67	123.70
22	BA	1900	A	N3-C4-C5	-9.96	119.82	126.80
22	BA	1937	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	1081	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	161	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	439	A	C5-C6-N6	9.96	131.67	123.70
22	BA	422	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	196	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	1333	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	226	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	945	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	2284	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	1722	A	C5-C6-N6	9.96	131.66	123.70
1	AA	236	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	599	A	C5-C6-N6	9.95	131.66	123.70
22	BA	602	A	C5-C6-N6	9.95	131.66	123.70
22	BA	1678	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	155	A	C5-C6-N6	9.95	131.66	123.70
1	AA	784	A	C5-C6-N6	9.95	131.66	123.70
22	BA	195	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	1978	A	C5-C6-N6	9.95	131.66	123.70
22	BA	2665	A	N3-C4-C5	-9.95	119.83	126.80
23	BB	59	A	N3-C4-N9	9.95	135.36	127.40
1	AA	262	A	N3-C4-C5	-9.95	119.84	126.80
1	AA	1256	A	C5-C6-N6	9.95	131.66	123.70
22	BA	1711	A	C5-C6-N6	9.94	131.66	123.70
1	AA	496	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1664	A	C5-C6-N6	9.94	131.65	123.70
22	BA	1969	A	C5-C6-N6	9.94	131.66	123.70
22	BA	829	A	N7-C8-N9	-9.94	108.83	113.80
1	AA	502	A	C5-C6-N6	9.94	131.65	123.70
22	BA	632	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1392	A	C5-C6-N6	9.94	131.65	123.70
22	BA	457	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1978	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2761	A	C5-C6-N6	9.94	131.65	123.70
22	BA	979	A	C5-C6-N6	9.94	131.65	123.70
22	BA	1383	A	C5-C6-N6	9.94	131.65	123.70
22	BA	443	A	C5-C6-N6	9.94	131.65	123.70
22	BA	1237	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2090	A	C5-C6-N6	9.94	131.65	123.70
1	AA	1437	A	N3-C4-C5	-9.93	119.85	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	149	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1754	A	N7-C8-N9	-9.93	108.83	113.80
22	BA	1757	A	C5-C6-N6	9.93	131.65	123.70
22	BA	2851	A	C5-C6-N6	9.93	131.65	123.70
22	BA	482	A	N7-C8-N9	-9.93	108.84	113.80
22	BA	507	A	C5-C6-N6	9.93	131.64	123.70
1	AA	602	A	C5-C6-N6	9.93	131.64	123.70
1	AA	1080	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	1429	A	C5-C6-N6	9.93	131.64	123.70
22	BA	221	A	N7-C8-N9	-9.93	108.84	113.80
22	BA	739	A	C5-C6-N6	9.93	131.64	123.70
22	BA	118	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1525	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	807	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	448	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1111	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	2095	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	2184	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	1229	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	917	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1739	A	C5-C6-N6	9.92	131.64	123.70
22	BA	1749	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	190	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	49	A	N3-C4-C5	-9.92	119.86	126.80
23	BB	39	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	947	A	C5-C6-N6	9.91	131.63	123.70
22	BA	1598	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	749	A	C5-C6-N6	9.91	131.63	123.70
1	AA	1170	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2270	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1247	A	C5-N7-C8	9.91	108.86	103.90
22	BA	2433	A	N3-C4-C5	-9.91	119.86	126.80
23	BB	59	A	C4-C5-C6	9.91	121.96	117.00
22	BA	21	A	C5-C6-N6	9.91	131.63	123.70
1	AA	1191	A	C5-C6-N6	9.91	131.63	123.70
1	AA	1418	A	C5-C6-N6	9.91	131.62	123.70
22	BA	83	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	609	A	N7-C8-N9	-9.91	108.85	113.80
22	BA	1175	A	C5-C6-N6	9.91	131.63	123.70
22	BA	2799	A	N3-C4-C5	-9.91	119.87	126.80
22	BA	309	A	C5-C6-N6	9.90	131.62	123.70
22	BA	1439	A	N3-C4-C5	-9.90	119.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1552	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	470	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	2311	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1265	A	C5-C6-N6	9.90	131.62	123.70
1	AA	825	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	541	A	C5-C6-N6	9.90	131.62	123.70
22	BA	1347	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	2893	A	N3-C4-C5	-9.90	119.87	126.80
55	B8	66	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	2108	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	1468	A	N3-C4-C5	-9.89	119.87	126.80
1	AA	706	A	C5-C6-N6	9.89	131.61	123.70
22	BA	941	A	N7-C8-N9	-9.89	108.86	113.80
1	AA	1410	A	N3-C4-C5	-9.89	119.88	126.80
22	BA	721	A	C5-C6-N6	9.89	131.61	123.70
22	BA	1427	A	N7-C8-N9	-9.89	108.86	113.80
1	AA	160	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	643	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	2829	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	109	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	2328	A	C5-C6-N6	9.88	131.60	123.70
1	AA	306	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	487	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	272	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	802	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	1241	A	C5-C6-N6	9.88	131.60	123.70
22	BA	1791	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	28	A	C5-C6-N6	9.88	131.60	123.70
1	AA	189	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	199	A	C5-C6-N6	9.88	131.60	123.70
22	BA	354	A	C5-C6-N6	9.88	131.60	123.70
22	BA	2516	A	N7-C8-N9	-9.88	108.86	113.80
1	AA	315	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1339	A	C5-C6-N6	9.88	131.60	123.70
22	BA	1953	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	415	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	609	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1360	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	340	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	149	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	780	A	C5-C6-N6	9.87	131.60	123.70
1	AA	702	A	C5-C6-N6	9.87	131.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1299	A	C5-C6-N6	9.87	131.60	123.70
22	BA	751	A	C5-C6-N6	9.87	131.60	123.70
22	BA	1086	A	C5-C6-N6	9.87	131.59	123.70
22	BA	299	A	N7-C8-N9	-9.87	108.87	113.80
22	BA	910	A	C5-C6-N6	9.87	131.59	123.70
1	AA	663	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	975	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	5	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	730	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1551	A	C5-C6-N6	9.87	131.59	123.70
22	BA	1847	A	N3-C4-C5	-9.86	119.89	126.80
22	BA	2587	A	C5-C6-N6	9.86	131.59	123.70
1	AA	81	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	282	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	602	A	N3-C4-C5	-9.86	119.90	126.80
55	B8	42	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	482	A	C5-C6-N6	9.86	131.58	123.70
1	AA	1513	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1531	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	820	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	901	A	N7-C8-N9	-9.85	108.87	113.80
22	BA	1502	A	C5-C6-N6	9.85	131.58	123.70
22	BA	1690	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	676	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1042	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	1603	A	C5-C6-N6	9.85	131.58	123.70
1	AA	465	A	C5-C6-N6	9.85	131.58	123.70
22	BA	1504	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	2333	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	792	A	C5-N7-C8	9.84	108.82	103.90
1	AA	860	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1176	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	2820	A	C5-C6-N6	9.84	131.57	123.70
1	AA	794	A	C5-C6-N6	9.84	131.57	123.70
1	AA	1000	A	C5-C6-N6	9.84	131.57	123.70
22	BA	501	A	C5-C6-N6	9.84	131.57	123.70
22	BA	1046	A	C5-C6-N6	9.84	131.57	123.70
22	BA	1808	A	C5-C6-N6	9.84	131.57	123.70
1	AA	59	A	C5-C6-N6	9.84	131.57	123.70
22	BA	1308	A	C5-N7-C8	9.84	108.82	103.90
1	AA	195	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	759	A	C5-N7-C8	9.83	108.82	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	10	A	C5-C6-N6	9.83	131.57	123.70
22	BA	71	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	739	A	N7-C8-N9	-9.83	108.88	113.80
22	BA	2088	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	74	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	422	A	N7-C8-N9	-9.83	108.89	113.80
22	BA	222	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1147	A	C5-C6-N6	9.83	131.56	123.70
22	BA	1070	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	1147	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	1307	A	C5-C6-N6	9.82	131.56	123.70
1	AA	1151	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1188	A	C5-C6-N6	9.82	131.56	123.70
22	BA	556	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	792	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1534	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	735	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	1871	A	C5-C6-N6	9.81	131.55	123.70
22	BA	2430	A	C2-N3-C4	9.81	115.50	110.60
22	BA	2513	A	N7-C8-N9	-9.81	108.89	113.80
22	BA	794	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	959	A	N7-C8-N9	-9.81	108.89	113.80
22	BA	2873	A	N7-C8-N9	-9.81	108.90	113.80
1	AA	964	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	391	A	C5-C6-N6	9.81	131.54	123.70
22	BA	2241	A	N3-C4-C5	-9.81	119.94	126.80
22	BA	529	A	C5-N7-C8	9.80	108.80	103.90
22	BA	980	A	C5-C6-N6	9.80	131.54	123.70
22	BA	2378	A	C5-C6-N6	9.80	131.54	123.70
22	BA	2800	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	607	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	146	A	C5-C6-N6	9.80	131.54	123.70
22	BA	1632	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	2826	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	814	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	64	A	C5-C6-N6	9.80	131.54	123.70
1	AA	1014	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	91	A	C5-C6-N6	9.79	131.54	123.70
22	BA	1735	A	C5-C6-N6	9.79	131.54	123.70
1	AA	263	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	712	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1019	A	N3-C4-C5	-9.79	119.95	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1434	A	C5-C6-N6	9.79	131.53	123.70
22	BA	1987	A	C8-N9-C4	9.79	109.72	105.80
22	BA	2733	A	C5-C6-N6	9.79	131.53	123.70
22	BA	909	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1532	A	C5-C6-N6	9.79	131.53	123.70
1	AA	1306	A	N3-C4-C5	-9.78	119.96	126.80
22	BA	2518	A	C5-N7-C8	9.78	108.79	103.90
1	AA	596	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1169	A	C5-C6-N6	9.78	131.52	123.70
22	BA	689	A	N3-C4-C5	-9.78	119.96	126.80
22	BA	936	A	C5-C6-N6	9.78	131.52	123.70
22	BA	2435	A	C5-N7-C8	9.78	108.79	103.90
22	BA	2598	A	C5-C6-N6	9.78	131.52	123.70
22	BA	95	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	642	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	1987	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2241	A	C5-C6-N6	9.77	131.52	123.70
22	BA	2660	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	629	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2298	A	C5-C6-N6	9.77	131.52	123.70
1	AA	533	A	C5-C6-N6	9.77	131.51	123.70
1	AA	1044	A	C5-C6-N6	9.77	131.51	123.70
1	AA	673	A	C5-C6-N6	9.77	131.51	123.70
22	BA	2287	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2700	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	790	A	C5-C6-N6	9.76	131.51	123.70
22	BA	1433	A	C5-C6-N6	9.76	131.51	123.70
1	AA	374	A	C5-C6-N6	9.76	131.51	123.70
22	BA	1755	A	C5-N7-C8	9.76	108.78	103.90
22	BA	1080	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	2019	A	C5-C6-N6	9.76	131.51	123.70
22	BA	677	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1280	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	2366	A	C5-C6-N6	9.75	131.50	123.70
22	BA	294	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	928	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1569	A	C5-C6-N6	9.74	131.50	123.70
1	AA	223	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	695	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1252	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	608	A	C5-C6-N6	9.74	131.49	123.70
22	BA	1214	A	N7-C8-N9	-9.74	108.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2014	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	53	A	C5-C6-N6	9.74	131.49	123.70
1	AA	155	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	535	A	C5-C6-N6	9.74	131.49	123.70
22	BA	199	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1654	A	C5-C6-N6	9.74	131.49	123.70
22	BA	2665	A	C5-N7-C8	9.74	108.77	103.90
22	BA	2587	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	19	A	C5-C6-N6	9.73	131.49	123.70
22	BA	1802	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	1496	A	C5-C6-N6	9.73	131.49	123.70
1	AA	909	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	1073	A	C5-C6-N6	9.73	131.48	123.70
22	BA	925	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	231	A	C5-C6-N6	9.72	131.48	123.70
1	AA	781	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	1129	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	1885	A	C5-C6-N6	9.72	131.48	123.70
23	BB	104	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	1147	A	C5-N7-C8	9.72	108.76	103.90
22	BA	1890	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	279	A	C5-C6-N6	9.72	131.47	123.70
22	BA	125	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	471	A	C5-N7-C8	9.72	108.76	103.90
22	BA	156	A	C5-C6-N6	9.72	131.47	123.70
22	BA	1784	A	C5-C6-N6	9.72	131.47	123.70
23	BB	115	A	C5-C6-N6	9.72	131.47	123.70
22	BA	1021	A	C5-N7-C8	9.71	108.76	103.90
22	BA	2734	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1374	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1570	A	C5-C6-N6	9.71	131.47	123.70
1	AA	600	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1044	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	973	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1937	A	C5-N7-C8	9.71	108.75	103.90
22	BA	782	A	N3-C4-C5	-9.71	120.01	126.80
1	AA	460	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	1127	A	C5-C6-N6	9.70	131.46	123.70
22	BA	1610	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	1431	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	181	A	N3-C4-C5	-9.69	120.01	126.80
22	BA	2392	A	N7-C8-N9	-9.70	108.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1794	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	2094	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	2335	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	946	A	C5-C6-N6	9.69	131.45	123.70
22	BA	508	A	C5-C6-N6	9.69	131.45	123.70
22	BA	1794	A	C5-C6-N6	9.69	131.45	123.70
1	AA	468	A	C5-C6-N6	9.68	131.45	123.70
1	AA	583	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	1413	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	756	A	C5-C6-N6	9.68	131.44	123.70
22	BA	1175	A	N7-C8-N9	-9.68	108.96	113.80
1	AA	718	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	2518	A	C5-C6-N6	9.68	131.44	123.70
22	BA	447	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	2267	A	C5-N7-C8	9.68	108.74	103.90
22	BA	825	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	925	A	C5-C6-N6	9.68	131.44	123.70
1	AA	7	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	63	A	C5-C6-N6	9.68	131.44	123.70
22	BA	1265	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1396	A	C5-C6-N6	9.67	131.44	123.70
22	BA	131	A	C5-C6-N6	9.67	131.44	123.70
22	BA	666	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	1302	A	C5-C6-N6	9.67	131.43	123.70
22	BA	1608	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	65	A	N3-C4-C5	-9.66	120.03	126.80
22	BA	126	A	N3-C4-C5	-9.66	120.03	126.80
1	AA	344	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	221	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1637	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2094	A	C5-C6-N6	9.66	131.43	123.70
22	BA	2809	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2589	A	C8-N9-C4	9.66	109.66	105.80
55	B8	51	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1000	A	C5-C6-N6	9.66	131.43	123.70
22	BA	2173	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2369	A	C5-C6-N6	9.66	131.43	123.70
1	AA	1176	A	C5-C6-N6	9.65	131.42	123.70
1	AA	1434	A	C5-C6-N6	9.65	131.42	123.70
22	BA	195	A	C5-C6-N6	9.65	131.42	123.70
22	BA	1253	A	N7-C8-N9	-9.65	108.97	113.80
1	AA	414	A	N3-C4-C5	-9.65	120.04	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1155	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	661	A	N3-C4-C5	-9.65	120.04	126.80
22	BA	1384	A	N3-C4-C5	-9.65	120.04	126.80
23	BB	119	A	C5-C6-N6	9.65	131.42	123.70
1	AA	892	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	866	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	1916	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	1256	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2366	A	N7-C8-N9	-9.64	108.98	113.80
1	AA	729	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	1877	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	1960	A	C5-C6-N6	9.64	131.41	123.70
22	BA	1960	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1324	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2614	A	C5-C6-N6	9.64	131.41	123.70
1	AA	1319	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1429	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1508	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1505	A	N3-C4-C5	-9.64	120.06	126.80
22	BA	429	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1866	A	C5-C6-N6	9.63	131.41	123.70
1	AA	69	G	N3-C4-C5	-9.63	123.78	128.60
1	AA	546	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1170	A	C5-C6-N6	9.63	131.41	123.70
23	BB	29	A	C5-C6-N6	9.63	131.41	123.70
23	BB	29	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	927	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	59	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	819	A	N3-C4-C5	-9.62	120.06	126.80
22	BA	820	A	N7-C8-N9	-9.62	108.99	113.80
1	AA	872	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	373	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	1275	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	270	A	C5-C6-N6	9.61	131.39	123.70
22	BA	793	A	N7-C8-N9	-9.61	108.99	113.80
22	BA	2564	A	N3-C4-C5	-9.61	120.07	126.80
23	BB	99	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	1179	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	793	A	C5-C6-N6	9.61	131.39	123.70
1	AA	655	A	C5-C6-N6	9.61	131.39	123.70
22	BA	346	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	497	A	N3-C4-C5	-9.61	120.07	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	980	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	1392	A	N3-C4-C5	-9.61	120.08	126.80
1	AA	860	A	C5-N7-C8	9.61	108.70	103.90
1	AA	919	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	13	A	N7-C8-N9	-9.60	109.00	113.80
1	AA	978	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	529	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	1191	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	1340	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	1347	A	C5-C6-N6	9.60	131.38	123.70
22	BA	2781	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	1502	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	279	A	N7-C8-N9	-9.60	109.00	113.80
22	BA	1637	A	C5-C6-N6	9.60	131.38	123.70
22	BA	960	A	N7-C8-N9	-9.60	109.00	113.80
1	AA	1067	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	983	A	C5-C6-N6	9.59	131.38	123.70
22	BA	324	A	C5-C6-N6	9.59	131.37	123.70
1	AA	74	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	1188	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	1597	A	C5-N7-C8	9.59	108.69	103.90
1	AA	116	A	OP1-P-O3'	-9.59	84.11	105.20
1	AA	1151	A	C5-C6-N6	9.59	131.37	123.70
22	BA	262	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	1133	A	C5-N7-C8	9.59	108.69	103.90
22	BA	2547	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	1552	A	C5-C6-N6	9.58	131.37	123.70
22	BA	1579	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	33	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	969	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	1434	A	N3-C4-C5	-9.58	120.10	126.80
22	BA	633	A	C5-C6-N6	9.58	131.36	123.70
22	BA	1928	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	2872	A	N9-C4-C5	9.57	109.63	105.80
22	BA	131	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	1265	A	N7-C8-N9	-9.57	109.02	113.80
22	BA	144	A	C5-C6-N6	9.57	131.35	123.70
22	BA	2171	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	119	A	C5-N7-C8	9.56	108.68	103.90
22	BA	1086	A	N7-C8-N9	-9.56	109.02	113.80
1	AA	431	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	279	A	N3-C4-C5	-9.56	120.11	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1499	A	C5-C6-N6	9.56	131.35	123.70
22	BA	272	A	C5-C6-N6	9.56	131.35	123.70
1	AA	574	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	1717	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	452	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	702	A	N7-C8-N9	-9.55	109.02	113.80
1	AA	787	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	990	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	1803	A	N7-C8-N9	-9.56	109.02	113.80
22	BA	2288	A	C5-C6-N6	9.56	131.34	123.70
22	BA	1126	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	1805	A	C5-N7-C8	9.55	108.68	103.90
22	BA	2899	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	635	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	253	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	1035	A	N7-C8-N9	-9.55	109.03	113.80
22	BA	256	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	844	A	C5-C6-N6	9.55	131.34	123.70
22	BA	2868	A	N7-C8-N9	-9.55	109.02	113.80
22	BA	804	A	C5-C6-N6	9.55	131.34	123.70
23	BB	101	A	C5-N7-C8	9.55	108.67	103.90
22	BA	6	A	N3-C4-C5	-9.55	120.12	126.80
1	AA	238	A	N3-C4-C5	-9.54	120.12	126.80
1	AA	913	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	1169	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	310	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	1570	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	2632	A	C5-N7-C8	9.54	108.67	103.90
1	AA	1441	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	104	A	C5-C6-N6	9.54	131.33	123.70
1	AA	487	A	C5-C6-N6	9.53	131.32	123.70
1	AA	694	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	483	A	C5-C6-N6	9.53	131.32	123.70
22	BA	644	A	C5-N7-C8	9.53	108.66	103.90
22	BA	699	A	C5-N7-C8	9.53	108.66	103.90
22	BA	2453	A	C5-C6-N6	9.53	131.32	123.70
22	BA	1020	A	N7-C8-N9	-9.53	109.04	113.80
22	BA	1871	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	1251	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	2037	A	C5-C6-N6	9.52	131.32	123.70
22	BA	2101	A	C5-C6-N6	9.52	131.32	123.70
23	BB	109	A	N3-C4-C5	-9.52	120.13	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1810	A	N7-C8-N9	-9.52	109.04	113.80
22	BA	2287	A	C5-C6-N6	9.52	131.32	123.70
22	BA	2051	A	N7-C8-N9	-9.52	109.04	113.80
1	AA	523	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	256	A	C5-C6-N6	9.52	131.31	123.70
22	BA	975	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	66	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	908	A	C5-C6-N6	9.52	131.31	123.70
22	BA	1260	A	C5-C6-N6	9.52	131.31	123.70
22	BA	2297	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	1055	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	1508	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	1630	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	449	A	C5-N7-C8	9.51	108.66	103.90
1	AA	172	A	N3-C4-C5	-9.51	120.14	126.80
1	AA	743	A	C5-C6-N6	9.51	131.31	123.70
22	BA	1652	A	C5-N7-C8	9.51	108.65	103.90
22	BA	2042	A	C8-N9-C4	9.51	109.60	105.80
1	AA	1180	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1785	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1089	A	C5-C6-N6	9.50	131.30	123.70
22	BA	2273	A	C5-N7-C8	9.50	108.65	103.90
22	BA	311	A	N3-C4-C5	-9.50	120.15	126.80
1	AA	432	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1098	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1616	A	C5-C6-N6	9.50	131.30	123.70
22	BA	819	A	C5-C6-N6	9.49	131.30	123.70
22	BA	975	A	C5-C6-N6	9.49	131.30	123.70
23	BB	34	A	C5-C6-N6	9.49	131.29	123.70
22	BA	1275	A	N3-C4-C5	-9.49	120.16	126.80
1	AA	397	A	N7-C8-N9	-9.49	109.06	113.80
1	AA	456	A	C5-C6-N6	9.49	131.29	123.70
1	AA	907	A	C5-C6-N6	9.49	131.29	123.70
22	BA	943	A	C5-C6-N6	9.49	131.29	123.70
22	BA	1393	A	N3-C4-C5	-9.49	120.16	126.80
1	AA	498	A	N3-C4-N9	9.49	134.99	127.40
1	AA	1093	A	N3-C4-C5	-9.49	120.16	126.80
1	AA	1101	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	503	A	C5-C6-N6	9.49	131.29	123.70
22	BA	761	A	C5-C6-N6	9.49	131.29	123.70
22	BA	1936	A	N7-C8-N9	-9.49	109.06	113.80
22	BA	2366	A	N3-C4-C5	-9.49	120.16	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1322	A	N3-C4-C5	-9.49	120.16	126.80
1	AA	1333	A	C5-N7-C8	9.48	108.64	103.90
22	BA	2346	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	2614	A	C4-C5-C6	9.48	121.74	117.00
22	BA	2749	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	753	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	1324	A	C5-C6-N6	9.48	131.28	123.70
22	BA	482	A	C4-C5-C6	9.48	121.74	117.00
22	BA	483	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	2198	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	1608	A	C5-C6-N6	9.48	131.28	123.70
22	BA	160	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	1689	A	N3-C4-C5	-9.48	120.17	126.80
1	AA	878	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	1428	A	C5-N7-C8	9.47	108.64	103.90
1	AA	1465	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	1307	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	2748	A	C5-C6-N6	9.47	131.28	123.70
1	AA	182	A	C5-C6-N6	9.47	131.28	123.70
1	AA	1318	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	2071	A	C5-C6-N6	9.47	131.28	123.70
1	AA	553	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	384	A	C5-C6-N6	9.47	131.28	123.70
22	BA	718	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	2352	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	831	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	480	A	N7-C8-N9	-9.46	109.07	113.80
22	BA	1610	A	C5-C6-N6	9.47	131.27	123.70
22	BA	563	A	N3-C4-C5	-9.46	120.17	126.80
22	BA	1470	A	N3-C4-C5	-9.46	120.17	126.80
22	BA	2142	A	C5-C6-N6	9.46	131.27	123.70
22	BA	2589	A	N3-C4-C5	-9.46	120.17	126.80
1	AA	139	A	C5-C6-N6	9.46	131.27	123.70
22	BA	829	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	1477	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	2851	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	26	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	120	A	C5-C6-N6	9.46	131.27	123.70
22	BA	2461	A	C5-C6-N6	9.46	131.26	123.70
22	BA	541	A	N3-C4-C5	-9.45	120.18	126.80
1	AA	309	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	1288	A	N3-C4-C5	-9.45	120.19	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	167	A	C5-C6-N6	9.45	131.26	123.70
22	BA	2590	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	2278	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	2070	A	C5-N7-C8	9.45	108.62	103.90
1	AA	958	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	352	A	N3-C4-C5	-9.44	120.19	126.80
1	AA	1394	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1084	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1593	A	C5-C6-N6	9.44	131.25	123.70
22	BA	430	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	503	A	N7-C8-N9	-9.43	109.08	113.80
22	BA	2052	A	C5-N7-C8	9.43	108.62	103.90
22	BA	739	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1570	A	N7-C8-N9	-9.43	109.09	113.80
22	BA	1641	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1927	A	N7-C8-N9	-9.43	109.09	113.80
1	AA	412	A	N3-C4-C5	-9.43	120.20	126.80
1	AA	1016	A	N3-C4-C5	-9.43	120.20	126.80
1	AA	608	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1490	A	C5-C6-N6	9.43	131.24	123.70
22	BA	1504	A	C5-C6-N6	9.43	131.24	123.70
22	BA	1586	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1596	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1301	A	C5-C6-N6	9.42	131.24	123.70
1	AA	383	A	C4-C5-C6	9.42	121.71	117.00
1	AA	648	A	N3-C4-C5	-9.42	120.20	126.80
1	AA	1130	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	1230	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	1858	A	C5-C6-N6	9.42	131.24	123.70
1	AA	435	A	N3-C4-C5	-9.41	120.21	126.80
23	BB	101	A	C4-C5-C6	9.41	121.71	117.00
22	BA	1676	A	C5-C6-N6	9.41	131.23	123.70
1	AA	8	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	129	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	1304	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	1872	A	C5-C6-N6	9.41	131.23	123.70
1	AA	802	A	C5-N7-C8	9.41	108.60	103.90
22	BA	2781	A	C5-C6-N6	9.41	131.23	123.70
23	BB	99	A	C5-N7-C8	9.41	108.60	103.90
22	BA	1650	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	572	A	N7-C8-N9	-9.40	109.10	113.80
1	AA	262	A	C5-C6-N6	9.40	131.22	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	974	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	1000	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	1204	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1469	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	2	A	N3-C4-C5	-9.39	120.22	126.80
1	AA	482	A	N3-C4-C5	-9.39	120.23	126.80
1	AA	1377	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	643	A	C5-C6-N6	9.39	131.21	123.70
22	BA	1385	A	C5-N7-C8	9.39	108.59	103.90
22	BA	1754	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	1829	A	C5-N7-C8	9.39	108.59	103.90
22	BA	2879	A	C5-C6-N6	9.39	131.21	123.70
22	BA	909	A	C5-C6-N6	9.39	131.21	123.70
22	BA	1672	A	C5-C6-N6	9.39	131.21	123.70
22	BA	2266	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	899	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	2211	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	756	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	1327	A	C5-C6-N6	9.38	131.21	123.70
22	BA	1698	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	2005	A	C5-C6-N6	9.38	131.21	123.70
22	BA	1952	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	2823	A	C5-N7-C8	9.38	108.59	103.90
1	AA	1332	A	C5-C6-N6	9.38	131.20	123.70
1	AA	1428	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	602	A	N3-C4-C5	-9.38	120.24	126.80
55	B8	69	A	C5-C6-N6	9.38	131.20	123.70
1	AA	649	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	1039	A	N3-C4-C5	-9.38	120.24	126.80
1	AA	533	A	C4-C5-C6	9.37	121.69	117.00
1	AA	994	A	C5-C6-N6	9.37	131.20	123.70
1	AA	72	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	849	A	N7-C8-N9	-9.37	109.11	113.80
22	BA	10	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	262	A	C5-N7-C8	9.37	108.58	103.90
22	BA	715	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	1127	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	353	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	863	A	C5-C6-N6	9.36	131.19	123.70
22	BA	1877	A	C5-C6-N6	9.36	131.19	123.70
1	AA	573	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	816	A	N3-C4-C5	-9.36	120.25	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	878	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	687	A	N3-C4-C5	-9.35	120.25	126.80
22	BA	42	A	C5-C6-N6	9.35	131.18	123.70
22	BA	2705	A	N7-C8-N9	-9.35	109.12	113.80
22	BA	2821	A	N3-C4-C5	-9.35	120.25	126.80
1	AA	1252	A	C5-C6-N6	9.35	131.18	123.70
22	BA	173	A	N3-C4-C5	-9.35	120.25	126.80
22	BA	470	A	C5-C6-N6	9.35	131.18	123.70
22	BA	391	A	C4-C5-C6	9.35	121.67	117.00
1	AA	502	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	477	A	C5-C6-N6	9.35	131.18	123.70
22	BA	1205	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	2447	G	C6-N1-C2	-9.35	119.49	125.10
1	AA	718	A	C5-C6-N6	9.35	131.18	123.70
22	BA	1616	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	1028	A	C5-C6-N6	9.34	131.18	123.70
1	AA	77	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	933	A	C5-N7-C8	9.34	108.57	103.90
1	AA	72	A	C5-C6-N6	9.34	131.17	123.70
1	AA	759	A	N3-C4-C5	-9.34	120.27	126.80
22	BA	191	A	C5-C6-N6	9.34	131.17	123.70
1	AA	1171	A	C5-C6-N6	9.33	131.17	123.70
22	BA	2266	A	N7-C8-N9	-9.33	109.13	113.80
22	BA	972	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	1367	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	2309	A	N3-C4-C5	-9.33	120.27	126.80
1	AA	1447	A	N3-C4-C5	-9.33	120.27	126.80
1	AA	1254	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	103	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	196	A	C5-N7-C8	9.33	108.56	103.90
22	BA	637	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	1214	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	2433	A	C5-C6-N6	9.33	131.16	123.70
1	AA	190	A	C5-C6-N6	9.32	131.16	123.70
1	AA	622	A	N3-C4-C5	-9.32	120.27	126.80
1	AA	768	A	C5-N7-C8	9.32	108.56	103.90
1	AA	747	A	C5-C6-N6	9.32	131.16	123.70
1	AA	937	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	941	A	C5-C6-N6	9.32	131.16	123.70
22	BA	2738	A	N3-C4-C5	-9.32	120.28	126.80
1	AA	1274	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	165	A	N3-C4-C5	-9.31	120.28	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2476	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	401	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	2468	A	C5-C6-N6	9.31	131.15	123.70
1	AA	749	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	914	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	1456	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	1496	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	794	A	N3-C4-C5	-9.31	120.29	126.80
22	BA	191	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	327	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	1169	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1284	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1679	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2247	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2071	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1616	A	N7-C8-N9	-9.30	109.15	113.80
22	BA	2560	A	C5-C6-N6	9.30	131.14	123.70
22	BA	251	A	N7-C8-N9	-9.30	109.15	113.80
22	BA	1069	A	C5-N7-C8	9.30	108.55	103.90
1	AA	533	A	C5-N7-C8	9.29	108.55	103.90
22	BA	1384	A	C5-C6-N6	9.29	131.14	123.70
22	BA	1508	A	C5-C6-N6	9.30	131.14	123.70
1	AA	1398	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	721	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1634	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	324	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	920	A	N3-C4-C5	-9.29	120.30	126.80
23	BB	101	A	N3-C4-N9	9.29	134.83	127.40
22	BA	1395	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	2135	A	N7-C8-N9	-9.28	109.16	113.80
22	BA	936	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	1553	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	466	A	C5-C6-N6	9.28	131.12	123.70
22	BA	609	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	900	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	1848	A	C5-C6-N6	9.28	131.12	123.70
23	BB	15	A	N3-C4-C5	-9.28	120.31	126.80
55	B8	58	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	1204	A	C5-N7-C8	9.27	108.54	103.90
22	BA	2327	A	C5-N7-C8	9.27	108.54	103.90
1	AA	69	G	N3-C4-N9	9.27	131.56	126.00
22	BA	218	A	N7-C8-N9	-9.27	109.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1590	A	C5-C6-N6	9.27	131.12	123.70
22	BA	1085	A	C5-N7-C8	9.27	108.53	103.90
22	BA	1759	A	C5-C6-N6	9.27	131.12	123.70
1	AA	767	A	C5-C6-N6	9.27	131.11	123.70
1	AA	1408	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	608	A	C5-N7-C8	9.26	108.53	103.90
22	BA	2705	A	N3-C4-C5	-9.26	120.31	126.80
22	BA	2670	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	626	A	C5-C6-N6	9.26	131.10	123.70
22	BA	1020	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	1918	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	2418	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	265	A	N3-C4-C5	-9.25	120.32	126.80
1	AA	303	A	N3-C4-C5	-9.25	120.32	126.80
1	AA	382	A	N3-C4-C5	-9.25	120.32	126.80
1	AA	878	A	C5-C6-N6	9.25	131.10	123.70
22	BA	251	A	C5-C6-N6	9.25	131.10	123.70
22	BA	2033	A	N3-C4-C5	-9.25	120.32	126.80
22	BA	1966	A	N3-C4-C5	-9.25	120.32	126.80
22	BA	2632	A	N3-C4-C5	-9.25	120.32	126.80
1	AA	1179	A	C5-N7-C8	9.25	108.52	103.90
22	BA	1503	A	C5-C6-N6	9.25	131.10	123.70
22	BA	1899	A	N3-C4-C5	-9.25	120.33	126.80
1	AA	10	A	C5-C6-N6	9.25	131.10	123.70
1	AA	1349	A	N3-C4-C5	-9.25	120.33	126.80
1	AA	1021	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	2020	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	2273	A	N3-C4-N9	9.24	134.79	127.40
22	BA	197	A	N7-C8-N9	-9.24	109.18	113.80
55	B8	38	A	N3-C4-C5	-9.24	120.33	126.80
1	AA	182	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	833	A	C5-C6-N6	9.23	131.09	123.70
22	BA	384	A	N3-C4-C5	-9.23	120.34	126.80
55	B8	6	A	N3-C4-C5	-9.23	120.34	126.80
55	B8	21	A	N3-C4-C5	-9.23	120.34	126.80
1	AA	872	A	N7-C8-N9	-9.23	109.19	113.80
1	AA	1261	A	C5-C6-N6	9.23	131.08	123.70
22	BA	244	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	1847	A	C5-C6-N6	9.23	131.08	123.70
22	BA	1977	A	C5-C6-N6	9.23	131.08	123.70
22	BA	218	A	N3-C4-C5	-9.22	120.34	126.80
22	BA	631	A	N3-C4-C5	-9.22	120.34	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	712	A	C5-C6-N6	9.22	131.08	123.70
22	BA	1664	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	2450	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	94	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	1346	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	149	A	N7-C8-N9	-9.21	109.19	113.80
22	BA	1509	A	N3-C4-C5	-9.21	120.35	126.80
1	AA	68	G	O4'-C1'-N9	9.21	115.57	108.20
1	AA	441	A	N3-C4-C5	-9.21	120.35	126.80
1	AA	918	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	943	A	N7-C8-N9	-9.21	109.19	113.80
22	BA	2598	A	N3-C4-C5	-9.21	120.35	126.80
1	AA	782	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	833	A	N3-C4-C5	-9.21	120.36	126.80
1	AA	338	A	C5-C6-N6	9.20	131.06	123.70
1	AA	1257	A	N3-C4-C5	-9.21	120.36	126.80
1	AA	1368	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	2392	A	N3-C4-C5	-9.20	120.36	126.80
23	BB	50	A	N3-C4-C5	-9.20	120.36	126.80
1	AA	1110	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	1803	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2058	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2412	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	608	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	1144	A	C8-N9-C4	9.20	109.48	105.80
22	BA	2386	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	28	A	N3-C4-C5	-9.19	120.36	126.80
22	BA	453	A	C5-C6-N6	9.20	131.06	123.70
22	BA	1413	A	N3-C4-C5	-9.19	120.36	126.80
22	BA	2430	A	N7-C8-N9	-9.19	109.20	113.80
1	AA	694	A	C5-C6-N6	9.19	131.05	123.70
1	AA	1004	A	C5-N7-C8	9.19	108.50	103.90
22	BA	2077	A	C5-C6-N6	9.19	131.05	123.70
22	BA	2407	A	N7-C8-N9	-9.19	109.21	113.80
22	BA	2516	A	N3-C4-C5	-9.19	120.37	126.80
55	B8	76	A	N7-C8-N9	-9.19	109.21	113.80
22	BA	181	A	N3-C4-C5	-9.18	120.37	126.80
1	AA	243	A	C5-N7-C8	9.18	108.49	103.90
1	AA	363	A	C5-N7-C8	9.18	108.49	103.90
1	AA	1271	A	N3-C4-C5	-9.18	120.37	126.80
1	AA	1513	A	C5-C6-N6	9.18	131.04	123.70
22	BA	2577	A	C5-N7-C8	9.18	108.49	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1250	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	466	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	1420	A	N3-C4-C5	-9.18	120.38	126.80
1	AA	872	A	C5-C6-N6	9.17	131.04	123.70
1	AA	1287	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	1593	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	2733	A	N3-C4-C5	-9.17	120.38	126.80
1	AA	119	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	479	A	C5-N7-C8	9.17	108.48	103.90
22	BA	1262	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	1787	A	C4-C5-C6	9.17	121.58	117.00
1	AA	192	A	C5-C6-N6	9.17	131.03	123.70
1	AA	228	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	727	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	996	A	C5-C6-N6	9.17	131.03	123.70
1	AA	1081	A	C5-C6-N6	9.16	131.03	123.70
22	BA	699	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	1260	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	1419	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	1470	A	C5-C6-N6	9.16	131.03	123.70
22	BA	1494	A	N3-C4-C5	-9.16	120.39	126.80
1	AA	1216	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	972	A	N7-C8-N9	-9.16	109.22	113.80
1	AA	329	A	C5-C6-N6	9.16	131.03	123.70
1	AA	579	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	727	A	C5-C6-N6	9.16	131.03	123.70
1	AA	320	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	599	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	2377	A	C5-C6-N6	9.15	131.02	123.70
1	AA	715	A	C5-C6-N6	9.15	131.02	123.70
22	BA	368	A	C5-C6-N6	9.15	131.02	123.70
22	BA	1772	A	N3-C4-C5	-9.15	120.39	126.80
1	AA	495	A	N3-C4-C5	-9.15	120.40	126.80
22	BA	83	A	C5-N7-C8	9.15	108.47	103.90
22	BA	1009	A	N3-C4-C5	-9.15	120.40	126.80
22	BA	1433	A	N3-C4-C5	-9.15	120.40	126.80
1	AA	1483	A	C5-C6-N6	9.14	131.01	123.70
1	AA	1499	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1244	A	C5-N7-C8	9.14	108.47	103.90
22	BA	666	A	C5-N7-C8	9.14	108.47	103.90
22	BA	685	A	N7-C8-N9	-9.14	109.23	113.80
22	BA	14	A	N3-C4-C5	-9.14	120.40	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	101	A	C4-C5-C6	9.14	121.57	117.00
22	BA	1757	A	C8-N9-C4	9.13	109.45	105.80
1	AA	923	A	C5-C6-N6	9.13	131.01	123.70
1	AA	539	A	C5-C6-N6	9.13	131.00	123.70
22	BA	734	A	C5-C6-N6	9.13	131.00	123.70
22	BA	2448	A	C5-N7-C8	9.13	108.47	103.90
1	AA	1150	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1014	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	2565	A	C5-N7-C8	9.13	108.46	103.90
22	BA	2589	A	C5-C6-N6	9.12	131.00	123.70
22	BA	1247	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	1755	A	N3-C4-C5	-9.12	120.42	126.80
1	AA	743	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	2013	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	1583	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	2727	A	C5-C6-N6	9.11	130.99	123.70
1	AA	336	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	73	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	1701	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	2882	A	N3-C4-C5	-9.11	120.42	126.80
23	BB	45	A	C5-N7-C8	9.11	108.45	103.90
22	BA	1155	A	C5-N7-C8	9.11	108.45	103.90
1	AA	161	A	C5-C6-N6	9.10	130.98	123.70
22	BA	2565	A	C5-C6-N6	9.10	130.98	123.70
22	BA	2873	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1591	A	C5-C6-N6	9.10	130.98	123.70
22	BA	1453	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	689	A	C5-N7-C8	9.09	108.45	103.90
22	BA	1276	A	C5-N7-C8	9.09	108.45	103.90
22	BA	979	A	C5-N7-C8	9.09	108.44	103.90
22	BA	2679	A	N3-C4-N9	9.09	134.67	127.40
23	BB	104	A	C5-C6-N6	9.09	130.97	123.70
22	BA	1580	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	983	A	N3-C4-C5	-9.08	120.44	126.80
1	AA	274	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	979	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	1354	A	C5-N7-C8	9.08	108.44	103.90
22	BA	1378	A	N3-C4-C5	-9.08	120.44	126.80
1	AA	1197	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	538	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	2482	A	C5-N7-C8	9.08	108.44	103.90
22	BA	1165	A	N3-C4-C5	-9.08	120.45	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1866	A	C8-N9-C4	9.08	109.43	105.80
22	BA	1268	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	2753	A	N3-C4-C5	-9.07	120.45	126.80
1	AA	1213	A	C5-N7-C8	9.07	108.44	103.90
1	AA	1299	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	161	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	788	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	2482	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	479	A	C8-N9-C4	9.07	109.43	105.80
22	BA	2097	A	C5-C6-N6	9.07	130.96	123.70
1	AA	1476	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	501	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	661	A	C5-N7-C8	9.07	108.43	103.90
22	BA	1246	A	C5-N7-C8	9.06	108.43	103.90
1	AA	1275	A	C5-N7-C8	9.06	108.43	103.90
22	BA	863	A	C8-N9-C4	9.06	109.43	105.80
1	AA	288	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	477	A	N3-C4-C5	-9.06	120.46	126.80
1	AA	1036	A	N3-C4-C5	-9.06	120.46	126.80
1	AA	1311	A	C5-C6-N6	9.06	130.95	123.70
22	BA	1580	A	C5-N7-C8	9.06	108.43	103.90
1	AA	68	G	N3-C4-N9	9.05	131.43	126.00
1	AA	964	A	C5-C6-N6	9.05	130.94	123.70
22	BA	1713	A	N3-C4-C5	-9.05	120.46	126.80
22	BA	2376	A	N3-C4-C5	-9.05	120.46	126.80
1	AA	371	A	N3-C4-C5	-9.05	120.46	126.80
1	AA	74	A	C5-N7-C8	9.05	108.42	103.90
22	BA	217	A	N3-C4-C5	-9.05	120.47	126.80
22	BA	1142	A	C5-N7-C8	9.05	108.42	103.90
22	BA	1569	A	N3-C4-C5	-9.05	120.47	126.80
1	AA	790	A	N3-C4-C5	-9.05	120.47	126.80
22	BA	749	A	C5-N7-C8	9.04	108.42	103.90
22	BA	905	A	C5-N7-C8	9.04	108.42	103.90
22	BA	2037	A	N3-C4-C5	-9.05	120.47	126.80
22	BA	1090	A	C5-C6-N6	9.04	130.93	123.70
22	BA	2126	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	2634	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	368	A	N3-C4-C5	-9.04	120.47	126.80
23	BB	73	A	C5-C6-N6	9.04	130.93	123.70
1	AA	1377	A	C5-N7-C8	9.04	108.42	103.90
22	BA	402	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	603	A	N3-C4-C5	-9.04	120.47	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1032	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	1762	A	N7-C8-N9	-9.04	109.28	113.80
22	BA	2654	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	2887	A	N3-C4-C5	-9.04	120.47	126.80
1	AA	353	A	C5-C6-N6	9.04	130.93	123.70
22	BA	2298	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	2886	A	C5-C6-N6	9.03	130.93	123.70
1	AA	270	A	C5-C6-N6	9.03	130.93	123.70
22	BA	241	A	N7-C8-N9	-9.03	109.28	113.80
22	BA	845	A	C5-N7-C8	9.03	108.42	103.90
22	BA	2426	A	C5-C6-N6	9.03	130.93	123.70
22	BA	1204	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	749	A	C8-N9-C4	9.03	109.41	105.80
22	BA	1009	A	C5-C6-N6	9.03	130.92	123.70
22	BA	1495	A	N3-C4-C5	-9.03	120.48	126.80
1	AA	119	A	C8-N9-C4	9.02	109.41	105.80
1	AA	554	A	N3-C4-C5	-9.02	120.48	126.80
1	AA	1362	A	N3-C4-C5	-9.02	120.48	126.80
22	BA	1287	A	C5-C6-N6	9.02	130.92	123.70
22	BA	1378	A	C5-N7-C8	9.02	108.41	103.90
22	BA	1745	A	N3-C4-C5	-9.02	120.49	126.80
22	BA	528	A	N7-C8-N9	-9.02	109.29	113.80
55	B8	73	A	N3-C4-C5	-9.02	120.49	126.80
22	BA	2600	A	N3-C4-C5	-9.01	120.49	126.80
1	AA	777	A	N3-C4-C5	-9.01	120.49	126.80
1	AA	441	A	C5-C6-N6	9.01	130.91	123.70
22	BA	1366	A	N3-C4-C5	-9.01	120.50	126.80
22	BA	1504	A	C5-N7-C8	9.01	108.40	103.90
23	BB	59	A	C5-C6-N1	9.01	122.20	117.70
1	AA	171	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	981	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	2530	A	N3-C4-C5	-9.00	120.50	126.80
1	AA	1092	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	2572	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	354	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	1640	A	N3-C4-C5	-9.00	120.50	126.80
1	AA	1248	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	2184	A	C5-C6-N6	9.00	130.90	123.70
22	BA	2725	A	C5-C6-N6	9.00	130.90	123.70
1	AA	608	A	C5-C6-N6	8.99	130.90	123.70
22	BA	1189	A	C5-N7-C8	8.99	108.40	103.90
1	AA	715	A	N3-C4-C5	-8.99	120.51	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	222	A	C5-N7-C8	8.99	108.40	103.90
22	BA	1165	A	C5-N7-C8	8.99	108.40	103.90
1	AA	300	A	C5-C6-N6	8.99	130.89	123.70
22	BA	2748	A	N3-C4-C5	-8.99	120.51	126.80
1	AA	98	A	C4-C5-C6	8.99	121.49	117.00
1	AA	704	A	N3-C4-C5	-8.99	120.51	126.80
22	BA	794	A	C5-C6-N6	8.99	130.89	123.70
22	BA	1809	A	C5-C6-N6	8.99	130.89	123.70
22	BA	2147	A	N3-C4-C5	-8.99	120.51	126.80
22	BA	2758	A	N3-C4-C5	-8.99	120.51	126.80
1	AA	408	A	C5-N7-C8	8.98	108.39	103.90
1	AA	572	A	C5-N7-C8	8.98	108.39	103.90
22	BA	1630	A	C5-N7-C8	8.98	108.39	103.90
22	BA	2270	A	C5-N7-C8	8.98	108.39	103.90
1	AA	1508	A	C5-C6-N6	8.98	130.88	123.70
1	AA	411	A	C5-C6-N6	8.97	130.88	123.70
1	AA	1227	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	270	A	N3-C4-C5	-8.97	120.52	126.80
1	AA	460	A	C5-C6-N6	8.97	130.88	123.70
22	BA	631	A	C5-N7-C8	8.97	108.39	103.90
22	BA	1722	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	2170	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	1848	A	C4-C5-C6	8.97	121.48	117.00
23	BB	101	A	C5-C6-N6	8.97	130.87	123.70
22	BA	1156	A	C5-C6-N6	8.96	130.87	123.70
1	AA	1105	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	1596	A	C5-C6-N6	8.96	130.87	123.70
1	AA	889	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	1655	A	N3-C4-C5	-8.96	120.53	126.80
1	AA	520	A	C5-N7-C8	8.96	108.38	103.90
1	AA	1016	A	C5-N7-C8	8.96	108.38	103.90
1	AA	309	A	C5-N7-C8	8.95	108.38	103.90
1	AA	1502	A	N3-C4-C5	-8.95	120.53	126.80
22	BA	2406	A	N3-C4-C5	-8.95	120.53	126.80
22	BA	2749	A	N7-C8-N9	-8.95	109.32	113.80
22	BA	2587	A	C5-N7-C8	8.95	108.38	103.90
1	AA	468	A	N3-C4-C5	-8.95	120.54	126.80
22	BA	1745	A	C5-C6-N6	8.94	130.85	123.70
22	BA	374	A	C5-N7-C8	8.94	108.37	103.90
22	BA	541	A	C5-N7-C8	8.94	108.37	103.90
22	BA	1431	A	C5-C6-N6	8.94	130.85	123.70
22	BA	1901	A	C5-C6-N6	8.94	130.85	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2322	A	N3-C4-C5	-8.94	120.54	126.80
1	AA	579	A	C5-C6-N6	8.94	130.85	123.70
1	AA	609	A	C5-C6-N6	8.94	130.85	123.70
22	BA	590	A	N3-C4-C5	-8.94	120.54	126.80
1	AA	1499	A	C8-N9-C4	8.94	109.38	105.80
22	BA	197	A	N3-C4-C5	-8.94	120.54	126.80
1	AA	1021	A	C5-N7-C8	8.93	108.37	103.90
22	BA	1762	A	N3-C4-C5	-8.93	120.55	126.80
22	BA	2886	A	N3-C4-C5	-8.93	120.55	126.80
1	AA	190	A	C4-C5-C6	8.93	121.47	117.00
1	AA	1105	A	C5-C6-N6	8.93	130.84	123.70
22	BA	227	A	N3-C4-C5	-8.93	120.55	126.80
22	BA	2176	A	C5-C6-N6	8.93	130.84	123.70
54	B7	9	A	C5-N7-C8	8.93	108.36	103.90
22	BA	227	A	C5-C6-N6	8.92	130.84	123.70
1	AA	640	A	N3-C4-C5	-8.92	120.56	126.80
22	BA	941	A	N3-C4-C5	-8.92	120.56	126.80
22	BA	1144	A	N3-C4-C5	-8.92	120.56	126.80
22	BA	1872	A	C4-C5-C6	8.92	121.46	117.00
22	BA	1095	A	C5-N7-C8	8.91	108.36	103.90
22	BA	1654	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	2900	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	2052	A	C5-C6-N6	8.91	130.83	123.70
1	AA	1197	A	C5-C6-N6	8.91	130.82	123.70
22	BA	2378	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	64	A	C5-N7-C8	8.90	108.35	103.90
22	BA	479	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	1551	A	C5-N7-C8	8.90	108.35	103.90
1	AA	554	A	C5-N7-C8	8.90	108.35	103.90
1	AA	1019	A	C5-C6-N6	8.90	130.82	123.70
1	AA	80	A	C5-C6-N6	8.90	130.82	123.70
22	BA	2051	A	C5-C6-N6	8.90	130.82	123.70
22	BA	2268	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	2740	A	N3-C4-C5	-8.90	120.57	126.80
1	AA	906	A	C5-C6-N6	8.89	130.82	123.70
22	BA	1503	A	C5-N7-C8	8.89	108.35	103.90
22	BA	457	A	C5-N7-C8	8.89	108.35	103.90
22	BA	2284	A	C5-C6-N6	8.89	130.81	123.70
1	AA	167	A	C5-C6-N6	8.89	130.81	123.70
1	AA	364	A	C5-N7-C8	8.89	108.34	103.90
22	BA	633	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	1641	A	C5-N7-C8	8.88	108.34	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2108	A	C5-C6-N6	8.89	130.81	123.70
1	AA	69	G	N3-C2-N2	8.88	126.12	119.90
1	AA	767	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	352	A	C5-N7-C8	8.88	108.34	103.90
22	BA	2453	A	N7-C8-N9	-8.88	109.36	113.80
22	BA	2726	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	2336	A	N3-C4-C5	-8.88	120.58	126.80
1	AA	430	A	C5-C6-N6	8.88	130.80	123.70
1	AA	1145	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	63	A	N3-C4-C5	-8.88	120.59	126.80
22	BA	1821	A	C5-N7-C8	8.88	108.34	103.90
22	BA	863	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	5	A	C5-C6-N6	8.87	130.79	123.70
1	AA	681	A	N3-C4-C5	-8.86	120.60	126.80
1	AA	1246	A	C5-N7-C8	8.86	108.33	103.90
22	BA	1858	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	959	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	1420	A	C5-N7-C8	8.86	108.33	103.90
1	AA	1269	A	N3-C4-C5	-8.85	120.60	126.80
22	BA	111	A	N3-C4-C5	-8.85	120.61	126.80
1	AA	1306	A	C5-N7-C8	8.85	108.32	103.90
1	AA	130	A	N3-C4-C5	-8.85	120.61	126.80
22	BA	2163	A	N3-C4-C5	-8.85	120.61	126.80
1	AA	250	A	N3-C4-C5	-8.84	120.61	126.80
1	AA	356	A	C5-C6-N6	8.84	130.77	123.70
1	AA	1332	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	1027	A	C5-C6-N6	8.84	130.77	123.70
1	AA	10	A	N3-C4-C5	-8.84	120.61	126.80
1	AA	55	A	C5-N7-C8	8.84	108.32	103.90
22	BA	91	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	1434	A	N3-C4-C5	-8.84	120.61	126.80
1	AA	246	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	412	A	C5-N7-C8	8.84	108.32	103.90
22	BA	2757	A	C4-C5-C6	8.84	121.42	117.00
22	BA	1040	A	C5-C6-N6	8.84	130.77	123.70
22	BA	1509	A	C5-N7-C8	8.84	108.32	103.90
22	BA	1977	A	N3-C4-C5	-8.83	120.62	126.80
1	AA	51	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	144	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	2469	A	C5-C6-N6	8.83	130.76	123.70
1	AA	1146	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	2872	A	N3-C4-C5	-8.83	120.62	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	393	A	N3-C4-C5	-8.82	120.62	126.80
22	BA	482	A	N3-C4-C5	-8.82	120.62	126.80
22	BA	1728	C	N3-C2-O2	-8.82	115.72	121.90
22	BA	1098	A	C5-N7-C8	8.82	108.31	103.90
22	BA	1253	A	N3-C4-C5	-8.82	120.63	126.80
22	BA	613	A	N3-C4-C5	-8.81	120.63	126.80
1	AA	356	A	C5-N7-C8	8.81	108.31	103.90
1	AA	1022	A	N3-C4-C5	-8.81	120.63	126.80
22	BA	1936	A	C4-C5-C6	8.81	121.41	117.00
1	AA	1502	A	C5-N7-C8	8.81	108.31	103.90
22	BA	1057	A	N3-C4-C5	-8.81	120.63	126.80
22	BA	988	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	1373	A	C5-C6-N6	8.80	130.74	123.70
22	BA	2154	A	C5-N7-C8	8.80	108.30	103.90
1	AA	19	A	C5-C6-N6	8.80	130.74	123.70
22	BA	1528	A	C5-C6-N6	8.80	130.74	123.70
22	BA	2837	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	2119	A	N3-C4-C5	-8.80	120.64	126.80
1	AA	162	A	C5-C6-N6	8.79	130.74	123.70
22	BA	374	A	C4-C5-C6	8.80	121.40	117.00
22	BA	111	A	C5-N7-C8	8.79	108.30	103.90
22	BA	1635	A	N3-C4-C5	-8.79	120.64	126.80
1	AA	78	A	C5-N7-C8	8.79	108.30	103.90
22	BA	2009	A	N3-C4-C5	-8.79	120.64	126.80
1	AA	1163	A	N3-C4-C5	-8.79	120.65	126.80
22	BA	1669	A	C5-N7-C8	8.79	108.30	103.90
22	BA	2450	A	C5-C6-N6	8.79	130.73	123.70
22	BA	2810	A	N3-C4-C5	-8.79	120.65	126.80
1	AA	197	A	N3-C4-C5	-8.78	120.65	126.80
1	AA	298	A	N3-C4-C5	-8.78	120.65	126.80
1	AA	510	A	N3-C4-C5	-8.79	120.65	126.80
22	BA	342	A	N3-C4-C5	-8.78	120.65	126.80
1	AA	1410	A	C5-N7-C8	8.78	108.29	103.90
22	BA	1194	A	C5-N7-C8	8.78	108.29	103.90
22	BA	422	A	C5-C6-N6	8.78	130.72	123.70
22	BA	2134	A	N3-C4-C5	-8.78	120.65	126.80
1	AA	996	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	1919	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	2469	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	2478	A	N3-C4-C5	-8.78	120.66	126.80
1	AA	546	A	C5-C6-N6	8.78	130.72	123.70
23	BB	119	A	N3-C4-C5	-8.78	120.66	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1969	A	N3-C4-C5	-8.77	120.66	126.80
22	BA	1802	A	N7-C8-N9	-8.76	109.42	113.80
22	BA	415	A	N3-C4-N9	8.76	134.41	127.40
22	BA	749	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	861	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	2856	A	C5-N7-C8	8.76	108.28	103.90
23	BB	94	A	C5-N7-C8	8.76	108.28	103.90
1	AA	1429	A	C5-N7-C8	8.76	108.28	103.90
22	BA	614	A	N3-C4-C5	-8.76	120.67	126.80
1	AA	935	A	C5-N7-C8	8.76	108.28	103.90
22	BA	586	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	789	A	C5-C6-N6	8.76	130.71	123.70
22	BA	415	A	C4-C5-C6	8.75	121.38	117.00
22	BA	1367	A	C5-N7-C8	8.75	108.28	103.90
22	BA	1596	A	C5-N7-C8	8.75	108.28	103.90
22	BA	2821	A	C8-N9-C4	8.75	109.30	105.80
23	BB	115	A	N3-C4-C5	-8.75	120.68	126.80
22	BA	685	A	C4-C5-C6	8.75	121.37	117.00
22	BA	2340	A	N3-C4-C5	-8.75	120.68	126.80
22	BA	2675	A	C5-N7-C8	8.74	108.27	103.90
1	AA	1157	A	C5-N7-C8	8.74	108.27	103.90
22	BA	2439	A	N3-C4-C5	-8.74	120.68	126.80
1	AA	179	A	N3-C4-C5	-8.74	120.68	126.80
1	AA	499	A	C5-N7-C8	8.73	108.27	103.90
22	BA	125	A	C5-N7-C8	8.73	108.27	103.90
1	AA	98	A	N3-C4-N9	8.73	134.38	127.40
1	AA	411	A	C8-N9-C4	8.73	109.29	105.80
22	BA	996	A	N3-C4-C5	-8.73	120.69	126.80
1	AA	1430	A	N3-C4-C5	-8.73	120.69	126.80
22	BA	216	A	N3-C4-C5	-8.73	120.69	126.80
22	BA	1998	A	C5-N7-C8	8.73	108.27	103.90
23	BB	78	A	N3-C4-C5	-8.73	120.69	126.80
22	BA	2758	A	C8-N9-C4	8.73	109.29	105.80
22	BA	1866	A	N3-C4-C5	-8.72	120.69	126.80
22	BA	582	A	N3-C4-C5	-8.72	120.69	126.80
22	BA	152	A	N3-C4-C5	-8.72	120.70	126.80
22	BA	1189	A	C5-C6-N6	8.72	130.68	123.70
1	AA	77	A	C5-N7-C8	8.72	108.26	103.90
1	AA	1503	A	C5-N7-C8	8.72	108.26	103.90
22	BA	2273	A	C4-C5-C6	8.72	121.36	117.00
22	BA	42	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	750	A	C5-N7-C8	8.72	108.26	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2183	A	C5-C6-N6	8.72	130.67	123.70
22	BA	2314	A	C5-N7-C8	8.72	108.26	103.90
22	BA	1711	A	N3-C4-C5	-8.71	120.70	126.80
23	BB	73	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	1784	A	C8-N9-C4	8.71	109.28	105.80
22	BA	2227	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	2358	A	N3-C4-C5	-8.71	120.70	126.80
1	AA	1418	A	C4-C5-C6	8.71	121.36	117.00
1	AA	1503	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	223	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	2273	A	C5-C6-N6	8.71	130.67	123.70
22	BA	2542	A	C5-N7-C8	8.71	108.25	103.90
22	BA	2600	A	C5-C6-N6	8.71	130.66	123.70
22	BA	119	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	716	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	1608	A	C8-N9-C4	8.70	109.28	105.80
22	BA	1772	A	C5-N7-C8	8.70	108.25	103.90
1	AA	243	A	N3-C4-C5	-8.70	120.71	126.80
1	AA	253	A	C5-N7-C8	8.70	108.25	103.90
22	BA	734	A	C8-N9-C4	8.70	109.28	105.80
22	BA	821	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	2602	A	C5-N7-C8	8.70	108.25	103.90
1	AA	16	A	N3-C4-C5	-8.69	120.72	126.80
1	AA	1503	A	C8-N9-C4	8.69	109.28	105.80
1	AA	1152	A	C5-C6-N6	8.69	130.65	123.70
22	BA	1336	A	C5-C6-N6	8.69	130.65	123.70
23	BB	109	A	C5-C6-N6	8.69	130.65	123.70
22	BA	1032	A	C5-N7-C8	8.69	108.24	103.90
22	BA	918	A	N3-C4-C5	-8.68	120.72	126.80
22	BA	1603	A	N3-C4-C5	-8.68	120.72	126.80
22	BA	603	A	C5-N7-C8	8.68	108.24	103.90
22	BA	2471	A	N3-C4-C5	-8.68	120.72	126.80
22	BA	2835	A	N3-C4-C5	-8.68	120.72	126.80
22	BA	1254	A	C5-N7-C8	8.68	108.24	103.90
22	BA	1359	A	N3-C4-C5	-8.68	120.73	126.80
22	BA	522	A	C5-C6-N6	8.68	130.64	123.70
22	BA	2459	A	C4-C5-C6	8.68	121.34	117.00
22	BA	2459	A	C5-C6-N6	8.68	130.64	123.70
1	AA	468	A	C5-N7-C8	8.67	108.24	103.90
22	BA	1548	A	C5-C6-N6	8.67	130.64	123.70
22	BA	28	A	N7-C8-N9	-8.67	109.47	113.80
22	BA	251	A	C4-C5-C6	8.67	121.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	655	A	C5-N7-C8	8.67	108.23	103.90
22	BA	1327	A	N3-C4-C5	-8.67	120.73	126.80
22	BA	1783	A	N3-C4-C5	-8.67	120.73	126.80
22	BA	2823	A	C8-N9-C4	8.67	109.27	105.80
22	BA	1089	A	N3-C4-C5	-8.66	120.73	126.80
22	BA	2860	A	N3-C4-C5	-8.66	120.73	126.80
1	AA	1105	A	C5-N7-C8	8.66	108.23	103.90
1	AA	1431	A	N3-C4-C5	-8.66	120.74	126.80
22	BA	1301	A	C5-N7-C8	8.66	108.23	103.90
22	BA	2900	A	C5-C6-N6	8.66	130.63	123.70
22	BA	1385	A	N3-C4-C5	-8.66	120.74	126.80
22	BA	1532	A	N3-C4-C5	-8.66	120.74	126.80
22	BA	2497	A	N7-C8-N9	-8.66	109.47	113.80
22	BA	2418	A	C5-N7-C8	8.65	108.23	103.90
22	BA	430	A	C5-N7-C8	8.65	108.23	103.90
22	BA	1021	A	C4-C5-C6	8.65	121.33	117.00
22	BA	825	A	C5-N7-C8	8.65	108.22	103.90
22	BA	1810	A	N3-C4-N9	8.65	134.32	127.40
1	AA	918	A	C5-N7-C8	8.64	108.22	103.90
1	AA	459	A	C5-C6-N6	8.64	130.61	123.70
22	BA	255	A	N3-C4-C5	-8.64	120.75	126.80
22	BA	52	A	N3-C4-C5	-8.64	120.75	126.80
1	AA	78	A	N3-C4-C5	-8.64	120.75	126.80
22	BA	764	A	N3-C4-C5	-8.64	120.75	126.80
22	BA	2080	A	C5-N7-C8	8.64	108.22	103.90
22	BA	718	A	C5-N7-C8	8.63	108.22	103.90
22	BA	1028	A	N3-C4-C5	-8.63	120.76	126.80
22	BA	1328	A	N3-C4-C5	-8.63	120.76	126.80
22	BA	1508	A	C5-N7-C8	8.63	108.22	103.90
1	AA	600	A	C5-N7-C8	8.63	108.22	103.90
22	BA	89	A	C5-N7-C8	8.63	108.22	103.90
22	BA	89	A	N3-C4-C5	-8.63	120.76	126.80
1	AA	687	A	C5-N7-C8	8.63	108.21	103.90
22	BA	1194	A	N3-C4-C5	-8.63	120.76	126.80
22	BA	1591	A	C5-N7-C8	8.62	108.21	103.90
1	AA	532	A	N3-C4-C5	-8.62	120.76	126.80
22	BA	213	A	N3-C4-C5	-8.62	120.77	126.80
22	BA	2758	A	C5-N7-C8	8.62	108.21	103.90
22	BA	1700	A	N3-C4-C5	-8.62	120.77	126.80
22	BA	1784	A	N3-C4-C5	-8.62	120.77	126.80
1	AA	441	A	C8-N9-C4	8.62	109.25	105.80
22	BA	877	A	C5-N7-C8	8.61	108.21	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1676	A	N7-C8-N9	-8.62	109.49	113.80
22	BA	2205	A	C5-N7-C8	8.62	108.21	103.90
1	AA	468	A	C8-N9-C4	8.61	109.25	105.80
1	AA	1167	A	N3-C4-C5	-8.61	120.77	126.80
1	AA	1227	A	N7-C8-N9	-8.61	109.49	113.80
22	BA	415	A	C5-C6-N6	8.61	130.59	123.70
22	BA	675	A	N3-C4-C5	-8.61	120.77	126.80
22	BA	1808	A	N3-C4-C5	-8.61	120.77	126.80
22	BA	575	A	N3-C4-C5	-8.61	120.77	126.80
22	BA	614	A	C8-N9-C4	8.61	109.24	105.80
1	AA	1102	A	C5-N7-C8	8.61	108.20	103.90
22	BA	1226	A	C5-N7-C8	8.61	108.20	103.90
22	BA	2750	A	C8-N9-C4	8.61	109.24	105.80
1	AA	563	A	C5-N7-C8	8.60	108.20	103.90
22	BA	167	A	C5-N7-C8	8.60	108.20	103.90
22	BA	505	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	282	A	C5-C6-N6	8.60	130.58	123.70
22	BA	820	A	C5-C6-N6	8.60	130.58	123.70
22	BA	2776	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	371	A	C5-N7-C8	8.60	108.20	103.90
22	BA	960	A	C5-N7-C8	8.60	108.20	103.90
22	BA	1272	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	1819	A	C5-N7-C8	8.60	108.20	103.90
22	BA	1677	A	N3-C4-C5	-8.60	120.78	126.80
23	BB	59	A	C5-N7-C8	8.59	108.20	103.90
1	AA	572	A	N3-C4-C5	-8.59	120.79	126.80
22	BA	126	A	C5-N7-C8	8.59	108.19	103.90
22	BA	1655	A	C5-N7-C8	8.59	108.19	103.90
1	AA	1285	A	C8-N9-C4	8.59	109.23	105.80
22	BA	2883	A	C5-N7-C8	8.59	108.19	103.90
1	AA	349	A	N3-C4-C5	-8.58	120.79	126.80
1	AA	547	A	C5-N7-C8	8.58	108.19	103.90
22	BA	2042	A	N3-C4-C5	-8.58	120.79	126.80
22	BA	2426	A	N3-C4-C5	-8.58	120.80	126.80
22	BA	1571	A	C5-N7-C8	8.57	108.19	103.90
22	BA	2042	A	C5-C6-N6	8.57	130.56	123.70
1	AA	149	A	C5-N7-C8	8.57	108.19	103.90
1	AA	1163	A	C5-C6-N6	8.57	130.56	123.70
22	BA	1001	A	N3-C4-C5	-8.57	120.80	126.80
1	AA	696	A	C5-N7-C8	8.57	108.18	103.90
1	AA	1502	A	C8-N9-C4	8.57	109.23	105.80
22	BA	592	A	N3-C4-C5	-8.57	120.80	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	892	A	C5-N7-C8	8.57	108.18	103.90
1	AA	349	A	C5-N7-C8	8.57	108.18	103.90
22	BA	1773	A	C5-C6-N6	8.57	130.55	123.70
22	BA	742	A	C5-C6-N6	8.56	130.55	123.70
22	BA	1050	A	C5-N7-C8	8.56	108.18	103.90
22	BA	2287	A	C4-C5-C6	8.56	121.28	117.00
22	BA	2211	A	C5-N7-C8	8.56	108.18	103.90
22	BA	2721	A	C5-C6-N6	8.56	130.54	123.70
22	BA	947	A	N3-C4-C5	-8.55	120.81	126.80
22	BA	1749	A	C5-N7-C8	8.56	108.18	103.90
22	BA	1854	A	C5-C6-N6	8.56	130.54	123.70
1	AA	246	A	C5-N7-C8	8.55	108.18	103.90
1	AA	535	A	N3-C4-C5	-8.55	120.81	126.80
22	BA	182	A	C5-N7-C8	8.55	108.18	103.90
22	BA	1029	A	N3-C4-C5	-8.55	120.81	126.80
22	BA	1144	A	C5-C6-N6	8.55	130.54	123.70
22	BA	1353	A	N3-C4-C5	-8.55	120.82	126.80
22	BA	2461	A	C5-N7-C8	8.55	108.17	103.90
22	BA	2740	A	C5-N7-C8	8.55	108.17	103.90
22	BA	705	A	C4-C5-C6	8.55	121.27	117.00
1	AA	300	A	N7-C8-N9	-8.54	109.53	113.80
22	BA	2163	A	C5-N7-C8	8.54	108.17	103.90
1	AA	1257	A	C5-N7-C8	8.54	108.17	103.90
22	BA	391	A	C5-N7-C8	8.54	108.17	103.90
23	BB	34	A	N3-C4-C5	-8.54	120.82	126.80
22	BA	515	A	C8-N9-C4	8.54	109.21	105.80
1	AA	1201	A	N3-C4-N9	8.53	134.23	127.40
1	AA	327	A	C5-N7-C8	8.53	108.17	103.90
1	AA	1289	A	N3-C4-C5	-8.53	120.83	126.80
1	AA	621	A	C5-N7-C8	8.53	108.17	103.90
22	BA	2792	A	C5-C6-N6	8.53	130.53	123.70
1	AA	1251	A	C5-N7-C8	8.53	108.16	103.90
22	BA	1626	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	2158	A	C5-N7-C8	8.53	108.16	103.90
22	BA	911	A	N7-C8-N9	-8.53	109.54	113.80
1	AA	167	A	C5-N7-C8	8.52	108.16	103.90
1	AA	1201	A	C4-C5-C6	8.52	121.26	117.00
1	AA	1480	A	N3-C4-C5	-8.52	120.83	126.80
22	BA	2095	A	C5-C6-N6	8.52	130.52	123.70
23	BB	52	A	N3-C4-C5	-8.52	120.83	126.80
1	AA	694	A	C5-N7-C8	8.52	108.16	103.90
22	BA	2241	A	C5-N7-C8	8.52	108.16	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	677	A	C5-N7-C8	8.51	108.16	103.90
22	BA	1014	A	C5-N7-C8	8.51	108.16	103.90
22	BA	1285	A	N3-C4-C5	-8.51	120.84	126.80
22	BA	2657	A	C8-N9-C4	8.51	109.20	105.80
22	BA	2721	A	N7-C8-N9	-8.51	109.54	113.80
1	AA	321	A	C5-N7-C8	8.51	108.15	103.90
22	BA	788	A	C5-N7-C8	8.51	108.15	103.90
1	AA	130	A	C8-N9-C4	8.50	109.20	105.80
1	AA	901	A	C5-C6-N6	8.50	130.50	123.70
1	AA	1340	A	C5-N7-C8	8.50	108.15	103.90
22	BA	1678	A	N3-C4-N9	8.50	134.20	127.40
22	BA	2333	A	C5-N7-C8	8.50	108.15	103.90
22	BA	627	A	C5-N7-C8	8.50	108.15	103.90
22	BA	1626	A	C5-C6-N6	8.50	130.50	123.70
22	BA	1545	A	N3-C4-C5	-8.50	120.85	126.80
22	BA	1566	A	C8-N9-C4	8.50	109.20	105.80
22	BA	1522	A	N3-C4-C5	-8.49	120.85	126.80
22	BA	1640	A	C5-N7-C8	8.49	108.14	103.90
22	BA	320	A	N3-C4-C5	-8.49	120.86	126.80
22	BA	344	A	N3-C4-C5	-8.49	120.86	126.80
22	BA	513	A	C5-C6-N6	8.49	130.49	123.70
22	BA	1528	A	C5-N7-C8	8.49	108.14	103.90
22	BA	173	A	C5-C6-N6	8.48	130.49	123.70
22	BA	1275	A	C8-N9-C4	8.48	109.19	105.80
22	BA	1728	C	C6-N1-C2	-8.48	116.91	120.30
22	BA	644	A	C4-C5-C6	8.48	121.24	117.00
22	BA	2682	A	N3-C4-C5	-8.48	120.86	126.80
22	BA	2766	A	C5-N7-C8	8.48	108.14	103.90
22	BA	204	A	N3-C4-C5	-8.48	120.87	126.80
1	AA	120	A	N3-C4-C5	-8.47	120.87	126.80
22	BA	2662	A	C4-C5-C6	8.47	121.24	117.00
22	BA	2778	A	C5-N7-C8	8.47	108.14	103.90
22	BA	1246	A	C5-C6-N6	8.47	130.48	123.70
1	AA	371	A	C5-N7-C8	8.47	108.13	103.90
1	AA	784	A	C5-N7-C8	8.47	108.13	103.90
1	AA	71	A	C5-N7-C8	8.46	108.13	103.90
22	BA	2632	A	C8-N9-C4	8.47	109.19	105.80
22	BA	1241	A	C4-C5-C6	8.46	121.23	117.00
22	BA	2821	A	C5-C6-N6	8.46	130.47	123.70
22	BA	1387	A	C5-N7-C8	8.46	108.13	103.90
1	AA	155	A	C5-N7-C8	8.46	108.13	103.90
22	BA	1652	A	N3-C4-C5	-8.46	120.88	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1966	A	C5-N7-C8	8.45	108.13	103.90
22	BA	2883	A	C8-N9-C4	8.45	109.18	105.80
1	AA	938	A	C4-C5-C6	8.45	121.23	117.00
1	AA	152	A	N3-C4-C5	-8.45	120.89	126.80
1	AA	1499	A	C5-N7-C8	8.45	108.12	103.90
22	BA	2054	A	C5-N7-C8	8.45	108.12	103.90
22	BA	52	A	C4-C5-C6	8.45	121.22	117.00
1	AA	236	A	C5-N7-C8	8.44	108.12	103.90
22	BA	654	A	C5-C6-N6	8.45	130.46	123.70
22	BA	1067	A	N3-C4-C5	-8.44	120.89	126.80
22	BA	1801	A	C5-N7-C8	8.45	108.12	103.90
22	BA	2060	A	N3-C4-C5	-8.45	120.89	126.80
1	AA	60	A	C4-C5-C6	8.44	121.22	117.00
22	BA	2821	A	C5-N7-C8	8.44	108.12	103.90
1	AA	814	A	C5-C6-N6	8.44	130.45	123.70
22	BA	155	A	C5-C6-N6	8.44	130.45	123.70
22	BA	1237	A	C5-N7-C8	8.44	108.12	103.90
22	BA	563	A	C5-N7-C8	8.43	108.12	103.90
22	BA	2430	A	C4-C5-C6	8.43	121.22	117.00
22	BA	2432	A	C5-C6-N6	8.43	130.44	123.70
22	BA	2872	A	C4-C5-N7	-8.43	106.48	110.70
22	BA	1365	A	C5-C6-N6	8.43	130.44	123.70
1	AA	238	A	C5-N7-C8	8.43	108.11	103.90
1	AA	1362	A	C5-N7-C8	8.43	108.11	103.90
22	BA	371	A	C8-N9-C4	8.43	109.17	105.80
22	BA	2757	A	N7-C8-N9	-8.43	109.59	113.80
22	BA	920	A	C5-C6-N6	8.43	130.44	123.70
1	AA	371	A	C5-C6-N6	8.42	130.44	123.70
1	AA	411	A	N3-C4-C5	-8.42	120.90	126.80
22	BA	415	A	C5-N7-C8	8.42	108.11	103.90
22	BA	1872	A	C5-N7-C8	8.42	108.11	103.90
1	AA	1493	A	C5-N7-C8	8.42	108.11	103.90
1	AA	1042	A	C5-N7-C8	8.42	108.11	103.90
22	BA	1938	A	C5-C6-N6	8.42	130.44	123.70
22	BA	1275	A	C5-N7-C8	8.42	108.11	103.90
22	BA	1175	A	C4-C5-C6	8.41	121.21	117.00
22	BA	2893	A	C5-N7-C8	8.41	108.11	103.90
22	BA	668	A	C5-N7-C8	8.41	108.11	103.90
22	BA	199	A	C5-N7-C8	8.40	108.10	103.90
22	BA	282	A	N3-C4-C5	-8.40	120.92	126.80
22	BA	1342	A	N3-C4-C5	-8.40	120.92	126.80
1	AA	81	A	C5-N7-C8	8.40	108.10	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1101	A	C5-N7-C8	8.40	108.10	103.90
22	BA	2883	A	N3-C4-C5	-8.40	120.92	126.80
1	AA	1446	A	C5-N7-C8	8.40	108.10	103.90
22	BA	1264	A	C5-C6-N6	8.40	130.42	123.70
22	BA	345	A	C5-N7-C8	8.39	108.10	103.90
22	BA	910	A	C8-N9-C4	8.39	109.16	105.80
22	BA	804	A	C5-N7-C8	8.39	108.10	103.90
22	BA	1700	A	C5-N7-C8	8.39	108.10	103.90
22	BA	1815	A	N3-C4-C5	-8.39	120.93	126.80
22	BA	2425	A	C5-N7-C8	8.39	108.10	103.90
22	BA	294	A	C5-N7-C8	8.39	108.09	103.90
22	BA	2657	A	N3-C4-C5	-8.39	120.93	126.80
22	BA	53	A	N3-C4-C5	-8.38	120.93	126.80
22	BA	2727	A	C4-C5-C6	8.39	121.19	117.00
22	BA	1889	A	C5-N7-C8	8.38	108.09	103.90
1	AA	815	A	C5-N7-C8	8.38	108.09	103.90
1	AA	493	A	N3-C4-C5	-8.38	120.93	126.80
1	AA	649	A	C5-N7-C8	8.38	108.09	103.90
22	BA	1548	A	N3-C4-C5	-8.38	120.93	126.80
1	AA	71	A	N3-C4-C5	-8.38	120.94	126.80
1	AA	746	A	C5-C6-N6	8.38	130.40	123.70
22	BA	574	A	C4-C5-C6	8.38	121.19	117.00
22	BA	616	A	C5-N7-C8	8.38	108.09	103.90
1	AA	845	A	C5-N7-C8	8.38	108.09	103.90
22	BA	670	A	C5-N7-C8	8.38	108.09	103.90
22	BA	2435	A	C8-N9-C4	8.38	109.15	105.80
22	BA	127	A	N3-C4-C5	-8.37	120.94	126.80
22	BA	2662	A	N7-C8-N9	-8.37	109.61	113.80
1	AA	1507	A	C5-C6-N6	8.37	130.40	123.70
22	BA	1175	A	N3-C4-N9	8.37	134.10	127.40
1	AA	1117	A	C8-N9-C4	8.37	109.15	105.80
22	BA	432	A	N3-C4-C5	-8.37	120.94	126.80
22	BA	2471	A	C5-C6-N6	8.37	130.40	123.70
22	BA	730	A	C5-C6-N6	8.37	130.39	123.70
22	BA	782	A	C5-N7-C8	8.37	108.08	103.90
1	AA	174	A	C5-N7-C8	8.37	108.08	103.90
22	BA	1321	A	C5-N7-C8	8.37	108.08	103.90
22	BA	2268	A	C5-N7-C8	8.37	108.08	103.90
1	AA	495	A	C5-N7-C8	8.36	108.08	103.90
1	AA	777	A	C5-N7-C8	8.37	108.08	103.90
22	BA	453	A	N3-C4-C5	-8.37	120.94	126.80
22	BA	2119	A	C5-N7-C8	8.37	108.08	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	866	A	C5-N7-C8	8.36	108.08	103.90
22	BA	2033	A	C5-N7-C8	8.36	108.08	103.90
1	AA	781	A	C8-N9-C4	8.36	109.14	105.80
1	AA	44	A	C5-N7-C8	8.36	108.08	103.90
22	BA	1073	A	N7-C8-N9	-8.36	109.62	113.80
1	AA	865	A	C5-N7-C8	8.36	108.08	103.90
1	AA	825	A	C5-N7-C8	8.35	108.08	103.90
22	BA	13	A	C4-C5-C6	8.35	121.17	117.00
1	AA	766	A	N3-C4-C5	-8.35	120.96	126.80
22	BA	191	A	C5-N7-C8	8.34	108.07	103.90
1	AA	389	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1918	A	C5-N7-C8	8.34	108.07	103.90
22	BA	2169	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1505	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1632	A	C5-N7-C8	8.34	108.07	103.90
22	BA	2082	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1970	A	C5-N7-C8	8.34	108.07	103.90
22	BA	2114	A	C5-N7-C8	8.34	108.07	103.90
1	AA	787	A	C5-N7-C8	8.33	108.07	103.90
22	BA	1650	A	C5-N7-C8	8.33	108.07	103.90
1	AA	1036	A	C5-N7-C8	8.33	108.07	103.90
22	BA	1143	A	C5-N7-C8	8.33	108.07	103.90
22	BA	1805	A	C5-C6-N1	8.33	121.87	117.70
22	BA	910	A	N3-C4-C5	-8.33	120.97	126.80
22	BA	990	A	C5-N7-C8	8.33	108.06	103.90
22	BA	278	A	C5-N7-C8	8.32	108.06	103.90
22	BA	38	A	C5-N7-C8	8.32	108.06	103.90
1	AA	1081	A	C5-N7-C8	8.32	108.06	103.90
22	BA	947	A	C5-N7-C8	8.32	108.06	103.90
22	BA	1490	A	C5-N7-C8	8.32	108.06	103.90
22	BA	1829	A	C4-C5-C6	8.32	121.16	117.00
22	BA	2411	A	N3-C4-C5	-8.32	120.98	126.80
22	BA	2826	A	C5-N7-C8	8.32	108.06	103.90
22	BA	1264	A	N3-C4-C5	-8.31	120.98	126.80
22	BA	1678	A	C5-C6-N6	8.31	130.35	123.70
22	BA	1286	A	N3-C4-C5	-8.31	120.98	126.80
22	BA	2879	A	C5-N7-C8	8.31	108.06	103.90
1	AA	675	A	N3-C4-C5	-8.31	120.98	126.80
22	BA	2670	A	C5-C6-N6	8.31	130.35	123.70
22	BA	572	A	C4-C5-C6	8.31	121.16	117.00
22	BA	1672	A	C8-N9-C4	8.31	109.12	105.80
22	BA	1853	A	N3-C4-C5	-8.31	120.98	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	919	A	C5-N7-C8	8.31	108.05	103.90
1	AA	1239	A	N3-C4-C5	-8.31	120.98	126.80
1	AA	673	A	C5-N7-C8	8.31	108.05	103.90
1	AA	746	A	C4-C5-C6	8.31	121.15	117.00
1	AA	977	A	C5-N7-C8	8.31	108.06	103.90
22	BA	2054	A	C5-C6-N6	8.31	130.35	123.70
1	AA	192	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1468	A	C5-C6-N6	8.31	130.34	123.70
1	AA	1480	A	C5-N7-C8	8.30	108.05	103.90
22	BA	1392	A	C5-N7-C8	8.31	108.05	103.90
22	BA	2225	A	N3-C4-C5	-8.31	120.99	126.80
23	BB	34	A	C5-N7-C8	8.30	108.05	103.90
1	AA	116	A	N3-C4-N9	8.30	134.04	127.40
1	AA	172	A	C5-N7-C8	8.30	108.05	103.90
22	BA	804	A	N3-C4-C5	-8.30	120.99	126.80
22	BA	1789	A	C5-N7-C8	8.30	108.05	103.90
22	BA	2531	A	C5-N7-C8	8.30	108.05	103.90
23	BB	50	A	C5-N7-C8	8.30	108.05	103.90
22	BA	142	A	C5-N7-C8	8.30	108.05	103.90
22	BA	783	A	N3-C4-N9	8.30	134.04	127.40
1	AA	753	A	C5-N7-C8	8.29	108.05	103.90
1	AA	498	A	C5-N7-C8	8.29	108.05	103.90
1	AA	1102	A	C5-C6-N6	8.29	130.33	123.70
22	BA	2287	A	C8-N9-C4	8.29	109.12	105.80
22	BA	371	A	N3-C4-C5	-8.29	121.00	126.80
1	AA	923	A	C4-C5-C6	8.29	121.14	117.00
22	BA	2274	A	N3-C4-C5	-8.29	121.00	126.80
1	AA	101	A	C4-C5-C6	8.29	121.14	117.00
1	AA	781	A	C5-N7-C8	8.29	108.04	103.90
22	BA	1791	A	C5-N7-C8	8.29	108.04	103.90
22	BA	2031	A	C5-N7-C8	8.29	108.04	103.90
1	AA	139	A	C5-N7-C8	8.28	108.04	103.90
1	AA	694	A	C8-N9-C4	8.28	109.11	105.80
22	BA	676	A	C8-N9-C4	8.28	109.11	105.80
1	AA	1346	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1046	A	C5-C6-N6	8.28	130.32	123.70
22	BA	71	A	C5-N7-C8	8.28	108.04	103.90
22	BA	927	A	C5-C6-N6	8.28	130.32	123.70
23	BB	58	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1374	A	C5-N7-C8	8.28	108.04	103.90
22	BA	256	A	C5-N7-C8	8.28	108.04	103.90
22	BA	1420	A	C8-N9-C4	8.27	109.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	938	A	C5-N7-C8	8.27	108.03	103.90
22	BA	1899	A	C4-C5-C6	8.27	121.14	117.00
1	AA	120	A	C8-N9-C4	8.27	109.11	105.80
22	BA	1583	A	C5-N7-C8	8.27	108.03	103.90
22	BA	2727	A	N3-C4-N9	8.27	134.01	127.40
1	AA	1196	A	N3-C4-C5	-8.27	121.01	126.80
22	BA	101	A	N3-C4-N9	8.27	134.01	127.40
22	BA	44	A	C5-N7-C8	8.27	108.03	103.90
1	AA	596	A	C5-N7-C8	8.26	108.03	103.90
22	BA	983	A	C8-N9-C4	8.26	109.11	105.80
22	BA	1247	A	N9-C4-C5	8.26	109.11	105.80
22	BA	1385	A	C8-N9-C4	8.26	109.11	105.80
1	AA	466	A	C5-N7-C8	8.26	108.03	103.90
22	BA	21	A	C5-N7-C8	8.26	108.03	103.90
1	AA	160	A	C5-N7-C8	8.25	108.03	103.90
22	BA	222	A	C8-N9-C4	8.25	109.10	105.80
22	BA	1544	A	C5-N7-C8	8.25	108.03	103.90
1	AA	746	A	N3-C4-N9	8.25	134.00	127.40
1	AA	864	A	C5-N7-C8	8.25	108.02	103.90
1	AA	1204	A	C5-N7-C8	8.25	108.02	103.90
22	BA	2287	A	C5-N7-C8	8.25	108.02	103.90
22	BA	2541	A	N3-C4-C5	-8.25	121.03	126.80
22	BA	863	A	C5-N7-C8	8.25	108.02	103.90
22	BA	1665	A	C5-N7-C8	8.24	108.02	103.90
22	BA	265	A	C5-N7-C8	8.24	108.02	103.90
22	BA	513	A	C4-C5-C6	8.24	121.12	117.00
22	BA	802	A	C5-N7-C8	8.24	108.02	103.90
22	BA	1393	A	C5-N7-C8	8.24	108.02	103.90
1	AA	274	A	C5-N7-C8	8.24	108.02	103.90
22	BA	821	A	C5-N7-C8	8.24	108.02	103.90
1	AA	602	A	C5-N7-C8	8.24	108.02	103.90
22	BA	626	A	N3-C4-C5	-8.24	121.03	126.80
22	BA	706	A	C5-N7-C8	8.24	108.02	103.90
22	BA	972	A	C5-C6-N6	8.24	130.29	123.70
22	BA	233	A	N3-C4-C5	-8.23	121.04	126.80
22	BA	1787	A	N3-C4-N9	8.23	133.99	127.40
22	BA	2013	A	C5-N7-C8	8.23	108.02	103.90
23	BB	66	A	C4-C5-C6	8.23	121.11	117.00
1	AA	279	A	N3-C4-C5	-8.23	121.04	126.80
1	AA	1413	A	C5-N7-C8	8.23	108.02	103.90
22	BA	53	A	C5-N7-C8	8.23	108.01	103.90
1	AA	315	A	C5-N7-C8	8.22	108.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	968	A	C5-N7-C8	8.22	108.01	103.90
22	BA	2451	A	C5-C6-N1	8.22	121.81	117.70
22	BA	526	A	C4-C5-C6	8.22	121.11	117.00
22	BA	2059	A	N3-C4-N9	8.22	133.97	127.40
23	BB	115	A	C5-N7-C8	8.22	108.01	103.90
22	BA	943	A	N3-C4-C5	-8.21	121.05	126.80
22	BA	878	A	C5-N7-C8	8.21	108.01	103.90
22	BA	1111	A	C5-N7-C8	8.21	108.01	103.90
22	BA	2407	A	N3-C4-N9	8.21	133.97	127.40
1	AA	143	A	N3-C4-C5	-8.21	121.05	126.80
1	AA	263	A	C5-N7-C8	8.21	108.00	103.90
1	AA	728	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1155	A	C5-N7-C8	8.21	108.00	103.90
22	BA	505	A	C5-N7-C8	8.21	108.00	103.90
22	BA	792	A	C5-N7-C8	8.21	108.00	103.90
22	BA	1133	A	N9-C4-C5	8.21	109.08	105.80
22	BA	1515	A	C5-N7-C8	8.21	108.00	103.90
22	BA	2879	A	N3-C4-N9	8.21	133.97	127.40
1	AA	1256	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1360	A	C5-N7-C8	8.21	108.00	103.90
22	BA	734	A	N3-C4-C5	-8.21	121.06	126.80
22	BA	1773	A	C4-C5-C6	8.20	121.10	117.00
22	BA	1866	A	C5-N7-C8	8.20	108.00	103.90
22	BA	1901	A	C4-C5-C6	8.21	121.10	117.00
22	BA	2082	A	C4-C5-C6	8.21	121.10	117.00
22	BA	1713	A	C5-N7-C8	8.20	108.00	103.90
22	BA	1787	A	C5-C6-N6	8.20	130.26	123.70
1	AA	994	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1280	A	C5-N7-C8	8.20	108.00	103.90
22	BA	917	A	C5-N7-C8	8.20	108.00	103.90
22	BA	2090	A	C5-N7-C8	8.20	108.00	103.90
22	BA	346	A	C5-N7-C8	8.20	108.00	103.90
22	BA	2346	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1465	A	C5-N7-C8	8.19	108.00	103.90
22	BA	1566	A	N3-C4-C5	-8.19	121.06	126.80
22	BA	2572	A	C5-N7-C8	8.20	108.00	103.90
22	BA	207	A	C5-N7-C8	8.19	108.00	103.90
22	BA	2317	A	C5-N7-C8	8.19	108.00	103.90
22	BA	1938	A	C5-N7-C8	8.19	107.99	103.90
22	BA	2741	A	N3-C4-C5	-8.19	121.07	126.80
22	BA	1912	A	C5-N7-C8	8.19	107.99	103.90
22	BA	5	A	C5-N7-C8	8.18	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	945	A	C5-N7-C8	8.18	107.99	103.90
22	BA	2173	A	C5-N7-C8	8.18	107.99	103.90
1	AA	7	A	C5-N7-C8	8.18	107.99	103.90
22	BA	443	A	N3-C4-C5	-8.18	121.07	126.80
22	BA	1637	A	C5-N7-C8	8.18	107.99	103.90
22	BA	2088	A	C5-N7-C8	8.18	107.99	103.90
22	BA	2800	A	C5-N7-C8	8.18	107.99	103.90
1	AA	539	A	C5-N7-C8	8.18	107.99	103.90
22	BA	522	A	N3-C4-N9	8.18	133.94	127.40
22	BA	866	A	C8-N9-C4	8.18	109.07	105.80
22	BA	1668	A	C5-N7-C8	8.18	107.99	103.90
55	B8	14	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1350	A	C5-N7-C8	8.17	107.99	103.90
1	AA	1375	A	C5-N7-C8	8.17	107.99	103.90
22	BA	1969	A	C4-C5-C6	8.17	121.09	117.00
1	AA	478	A	C5-N7-C8	8.17	107.98	103.90
1	AA	520	A	N3-C4-C5	-8.17	121.08	126.80
1	AA	430	A	C5-N7-C8	8.17	107.98	103.90
1	AA	32	A	C5-C6-N6	8.17	130.23	123.70
22	BA	515	A	N3-C4-C5	-8.17	121.08	126.80
22	BA	1269	A	C5-N7-C8	8.17	107.98	103.90
22	BA	2077	A	C5-N7-C8	8.17	107.98	103.90
1	AA	712	A	C5-N7-C8	8.16	107.98	103.90
1	AA	250	A	C5-N7-C8	8.16	107.98	103.90
22	BA	118	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1054	A	C5-C6-N6	8.16	130.23	123.70
22	BA	1634	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1171	A	C5-N7-C8	8.16	107.98	103.90
22	BA	529	A	N9-C4-C5	8.16	109.06	105.80
22	BA	1312	U	C5-C4-O4	8.16	130.80	125.90
22	BA	1876	A	C5-N7-C8	8.16	107.98	103.90
1	AA	189	A	C5-N7-C8	8.16	107.98	103.90
22	BA	522	A	C5-N7-C8	8.16	107.98	103.90
1	AA	383	A	C5-N7-C8	8.16	107.98	103.90
22	BA	753	A	C5-N7-C8	8.16	107.98	103.90
22	BA	782	A	C4-C5-C6	8.16	121.08	117.00
22	BA	2381	A	N3-C4-C5	-8.15	121.09	126.80
22	BA	1900	A	C5-N7-C8	8.15	107.98	103.90
55	B8	74	C	OP1-P-O3'	-8.15	87.26	105.20
22	BA	574	A	C5-N7-C8	8.15	107.98	103.90
22	BA	2199	A	C5-N7-C8	8.15	107.97	103.90
1	AA	665	A	N3-C4-C5	-8.15	121.10	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	325	A	C5-N7-C8	8.15	107.97	103.90
1	AA	313	A	C5-N7-C8	8.14	107.97	103.90
22	BA	532	A	C5-N7-C8	8.14	107.97	103.90
22	BA	1247	A	C4-C5-N7	-8.14	106.63	110.70
22	BA	547	A	C5-N7-C8	8.14	107.97	103.90
22	BA	722	A	C5-C6-N6	8.14	130.21	123.70
22	BA	2062	A	N3-C4-C5	-8.14	121.10	126.80
22	BA	272	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1513	A	C5-N7-C8	8.14	107.97	103.90
1	AA	498	A	C4-C5-C6	8.13	121.07	117.00
1	AA	1067	A	C5-N7-C8	8.14	107.97	103.90
22	BA	330	A	C5-N7-C8	8.14	107.97	103.90
22	BA	2589	A	C5-N7-C8	8.13	107.97	103.90
1	AA	383	A	C5-C6-N6	8.13	130.21	123.70
1	AA	546	A	C8-N9-C4	8.13	109.05	105.80
22	BA	1272	A	C8-N9-C4	8.13	109.05	105.80
23	BB	75	G	C6-N1-C2	-8.13	120.22	125.10
1	AA	131	A	C5-N7-C8	8.12	107.96	103.90
22	BA	278	A	C4-C5-C6	8.13	121.06	117.00
1	AA	1248	A	C5-N7-C8	8.12	107.96	103.90
22	BA	2600	A	C5-C6-N1	8.12	121.76	117.70
1	AA	130	A	C5-C6-N6	8.12	130.19	123.70
22	BA	472	A	N3-C4-C5	-8.12	121.12	126.80
1	AA	1180	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1285	A	C5-N7-C8	8.12	107.96	103.90
22	BA	1010	A	N3-C4-C5	-8.11	121.12	126.80
1	AA	414	A	C5-N7-C8	8.11	107.95	103.90
22	BA	1336	A	C5-N7-C8	8.11	107.95	103.90
22	BA	1739	A	C4-C5-C6	8.11	121.05	117.00
22	BA	756	A	C5-N7-C8	8.11	107.95	103.90
22	BA	743	A	C5-C6-N6	8.10	130.18	123.70
22	BA	1129	A	C5-N7-C8	8.10	107.95	103.90
1	AA	383	A	N3-C4-N9	8.10	133.88	127.40
1	AA	509	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1396	A	C4-C5-C6	8.10	121.05	117.00
23	BB	45	A	C4-C5-C6	8.10	121.05	117.00
22	BA	2117	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1329	A	N3-C4-C5	-8.10	121.13	126.80
22	BA	348	A	N3-C4-C5	-8.10	121.13	126.80
22	BA	1046	A	N3-C4-C5	-8.10	121.13	126.80
22	BA	1672	A	C5-N7-C8	8.10	107.95	103.90
22	BA	309	A	C5-N7-C8	8.09	107.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1213	A	N3-C4-N9	8.09	133.87	127.40
22	BA	1676	A	N3-C4-C5	-8.09	121.14	126.80
22	BA	2823	A	N3-C4-N9	8.09	133.87	127.40
1	AA	1408	A	C5-N7-C8	8.09	107.95	103.90
22	BA	1453	A	C5-N7-C8	8.09	107.94	103.90
22	BA	1829	A	N3-C4-N9	8.09	133.87	127.40
1	AA	182	A	C8-N9-C4	8.09	109.03	105.80
22	BA	2227	A	C5-N7-C8	8.09	107.94	103.90
22	BA	2837	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1476	A	C5-N7-C8	8.09	107.94	103.90
22	BA	668	A	N3-C4-C5	-8.09	121.14	126.80
22	BA	896	A	C5-N7-C8	8.09	107.94	103.90
22	BA	423	A	N3-C4-C5	-8.08	121.14	126.80
22	BA	2598	A	C4-C5-C6	8.08	121.04	117.00
22	BA	204	A	C5-N7-C8	8.08	107.94	103.90
22	BA	190	A	N7-C8-N9	-8.08	109.76	113.80
22	BA	984	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1134	A	C5-N7-C8	8.08	107.94	103.90
22	BA	2750	A	C5-N7-C8	8.08	107.94	103.90
22	BA	2879	A	C4-C5-C6	8.08	121.04	117.00
1	AA	393	A	C5-N7-C8	8.07	107.94	103.90
1	AA	152	A	C5-N7-C8	8.07	107.94	103.90
22	BA	735	A	C5-N7-C8	8.07	107.94	103.90
22	BA	1937	A	C4-C5-N7	-8.07	106.67	110.70
22	BA	401	A	C5-C6-N6	8.07	130.15	123.70
1	AA	116	A	C4-C5-C6	8.07	121.03	117.00
22	BA	2432	A	N3-C4-C5	-8.07	121.15	126.80
22	BA	2711	A	N3-C4-C5	-8.07	121.15	126.80
22	BA	1274	A	C5-N7-C8	8.06	107.93	103.90
1	AA	759	A	C8-N9-C4	8.06	109.03	105.80
22	BA	1717	A	C5-N7-C8	8.06	107.93	103.90
22	BA	2725	A	N3-C4-C5	-8.06	121.16	126.80
22	BA	362	A	C5-N7-C8	8.06	107.93	103.90
1	AA	996	A	C5-N7-C8	8.06	107.93	103.90
22	BA	1928	A	C5-N7-C8	8.05	107.93	103.90
22	BA	2386	A	C5-N7-C8	8.06	107.93	103.90
22	BA	2468	A	N3-C4-C5	-8.06	121.16	126.80
22	BA	2682	A	C5-C6-N6	8.06	130.15	123.70
22	BA	172	A	C5-N7-C8	8.05	107.93	103.90
22	BA	2682	A	C8-N9-C4	8.05	109.02	105.80
22	BA	514	A	N3-C4-C5	-8.05	121.16	126.80
22	BA	340	A	C5-N7-C8	8.05	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	515	A	C5-N7-C8	8.05	107.92	103.90
1	AA	19	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1534	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1285	A	C5-N7-C8	8.05	107.92	103.90
22	BA	52	A	C5-N7-C8	8.04	107.92	103.90
22	BA	439	A	C5-N7-C8	8.04	107.92	103.90
22	BA	507	A	N3-C4-C5	-8.04	121.17	126.80
22	BA	804	A	C8-N9-C4	8.04	109.02	105.80
22	BA	2829	A	C8-N9-C4	8.04	109.02	105.80
1	AA	974	A	C5-N7-C8	8.04	107.92	103.90
22	BA	983	A	C5-C6-N6	8.04	130.13	123.70
22	BA	2126	A	C5-N7-C8	8.04	107.92	103.90
1	AA	8	A	C5-N7-C8	8.04	107.92	103.90
1	AA	831	A	C5-N7-C8	8.04	107.92	103.90
22	BA	689	A	C8-N9-C4	8.04	109.02	105.80
1	AA	101	A	C4-C5-N7	-8.04	106.68	110.70
22	BA	2340	A	C5-C6-N6	8.04	130.13	123.70
42	BU	52	LEU	CA-CB-CG	8.04	133.78	115.30
22	BA	101	A	C5-N7-C8	8.03	107.92	103.90
22	BA	2719	G	C2-N3-C4	-8.04	107.88	111.90
22	BA	2882	A	C5-N7-C8	8.04	107.92	103.90
1	AA	143	A	C8-N9-C4	8.03	109.01	105.80
1	AA	648	A	C5-N7-C8	8.03	107.92	103.90
22	BA	2850	A	C5-N7-C8	8.03	107.92	103.90
22	BA	84	A	N3-C4-C5	-8.03	121.18	126.80
22	BA	231	A	C5-N7-C8	8.03	107.92	103.90
23	BB	53	A	C5-N7-C8	8.03	107.92	103.90
22	BA	1652	A	C8-N9-C4	8.03	109.01	105.80
22	BA	2727	A	C5-N7-C8	8.03	107.91	103.90
1	AA	595	A	C5-N7-C8	8.03	107.91	103.90
1	AA	1117	A	N3-C4-C5	-8.03	121.18	126.80
22	BA	103	A	C5-N7-C8	8.03	107.91	103.90
22	BA	900	A	C5-N7-C8	8.03	107.91	103.90
22	BA	1070	A	C5-N7-C8	8.03	107.91	103.90
22	BA	322	A	C5-N7-C8	8.02	107.91	103.90
22	BA	2335	A	C4-C5-C6	8.02	121.01	117.00
22	BA	2726	A	C5-N7-C8	8.02	107.91	103.90
1	AA	1368	A	C5-N7-C8	8.02	107.91	103.90
1	AA	270	A	C5-N7-C8	8.02	107.91	103.90
1	AA	792	A	C8-N9-C4	8.02	109.01	105.80
1	AA	860	A	C4-C5-C6	8.02	121.01	117.00
22	BA	6	A	C5-N7-C8	8.01	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	538	A	C5-N7-C8	8.01	107.91	103.90
22	BA	2059	A	C4-C5-C6	8.01	121.00	117.00
22	BA	2225	A	C5-N7-C8	8.01	107.91	103.90
22	BA	2565	A	C4-C5-C6	8.01	121.00	117.00
22	BA	2675	A	N3-C4-N9	8.01	133.81	127.40
1	AA	50	A	C5-N7-C8	8.00	107.90	103.90
22	BA	1469	A	C5-N7-C8	8.00	107.90	103.90
1	AA	1492	A	C5-N7-C8	8.00	107.90	103.90
22	BA	2761	A	C5-N7-C8	8.00	107.90	103.90
1	AA	959	A	C5-N7-C8	8.00	107.90	103.90
1	AA	430	A	C4-C5-C6	8.00	121.00	117.00
1	AA	1012	A	C5-N7-C8	8.00	107.90	103.90
1	AA	162	A	C4-C5-C6	7.99	121.00	117.00
22	BA	1854	A	N3-C4-N9	7.99	133.79	127.40
22	BA	156	A	C5-N7-C8	7.99	107.90	103.90
22	BA	1677	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1311	A	C5-N7-C8	7.99	107.89	103.90
22	BA	2171	A	C5-N7-C8	7.99	107.89	103.90
22	BA	522	A	C4-C5-C6	7.99	120.99	117.00
54	B7	10	U	O5'-P-OP2	7.99	120.28	110.70
1	AA	675	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1201	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1213	A	N3-C4-C5	-7.99	121.21	126.80
22	BA	492	A	C5-N7-C8	7.99	107.89	103.90
22	BA	1916	A	C5-N7-C8	7.99	107.89	103.90
22	BA	1276	A	C4-C5-C6	7.98	120.99	117.00
22	BA	2679	A	C5-C6-N6	7.98	130.09	123.70
1	AA	915	A	C8-N9-C4	7.98	108.99	105.80
1	AA	1429	A	C8-N9-C4	7.98	108.99	105.80
22	BA	1977	A	C8-N9-C4	7.98	108.99	105.80
22	BA	2297	A	C5-N7-C8	7.98	107.89	103.90
1	AA	1236	A	C5-C6-N6	7.98	130.09	123.70
1	AA	228	A	C5-N7-C8	7.98	107.89	103.90
1	AA	1500	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1591	A	C8-N9-C4	7.98	108.99	105.80
22	BA	2810	A	C5-N7-C8	7.98	107.89	103.90
22	BA	482	A	C5-C6-N6	7.98	130.08	123.70
22	BA	2589	A	N3-C4-N9	7.97	133.78	127.40
1	AA	1111	A	C5-N7-C8	7.97	107.89	103.90
22	BA	282	A	C5-N7-C8	7.97	107.88	103.90
1	AA	28	A	C5-N7-C8	7.96	107.88	103.90
22	BA	447	A	C5-N7-C8	7.96	107.88	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2600	A	C8-N9-C4	7.96	108.98	105.80
22	BA	2734	A	C5-N7-C8	7.96	107.88	103.90
1	AA	129	A	C5-N7-C8	7.96	107.88	103.90
1	AA	907	A	C5-N7-C8	7.96	107.88	103.90
22	BA	614	A	C5-N7-C8	7.96	107.88	103.90
1	AA	559	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1711	A	C5-N7-C8	7.96	107.88	103.90
22	BA	2287	A	N3-C4-N9	7.96	133.76	127.40
22	BA	2033	A	N9-C4-C5	7.95	108.98	105.80
22	BA	2468	A	C8-N9-C4	7.95	108.98	105.80
1	AA	1441	A	C5-N7-C8	7.95	107.88	103.90
22	BA	1690	A	C5-N7-C8	7.95	107.88	103.90
1	AA	819	A	C5-N7-C8	7.95	107.88	103.90
22	BA	1084	A	C5-N7-C8	7.95	107.88	103.90
22	BA	2281	A	N3-C4-C5	-7.95	121.23	126.80
1	AA	1398	A	C5-N7-C8	7.95	107.87	103.90
22	BA	466	A	C5-N7-C8	7.95	107.87	103.90
22	BA	722	A	C5-N7-C8	7.95	107.87	103.90
55	B8	73	A	C5-N7-C8	7.95	107.87	103.90
1	AA	10	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1885	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1722	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1937	A	N9-C4-C5	7.94	108.98	105.80
1	AA	1285	A	N3-C4-C5	-7.94	121.24	126.80
1	AA	1319	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1528	A	C4-C5-C6	7.94	120.97	117.00
22	BA	2602	A	N3-C4-C5	-7.94	121.24	126.80
22	BA	2376	A	C5-N7-C8	7.94	107.87	103.90
1	AA	344	A	C5-N7-C8	7.93	107.87	103.90
22	BA	502	A	C5-N7-C8	7.93	107.87	103.90
22	BA	1609	A	C5-N7-C8	7.93	107.87	103.90
1	AA	459	A	C5-N7-C8	7.93	107.87	103.90
22	BA	844	A	N3-C4-C5	-7.93	121.25	126.80
1	AA	1363	A	C5-N7-C8	7.93	107.87	103.90
22	BA	2670	A	C5-N7-C8	7.93	107.86	103.90
1	AA	1396	A	C5-N7-C8	7.93	107.86	103.90
22	BA	176	A	N3-C4-N9	7.93	133.74	127.40
22	BA	1614	A	C5-C6-N6	7.93	130.04	123.70
22	BA	721	A	C8-N9-C4	7.93	108.97	105.80
22	BA	311	A	C5-N7-C8	7.93	107.86	103.90
22	BA	1046	A	C8-N9-C4	7.93	108.97	105.80
22	BA	1551	A	C4-C5-C6	7.93	120.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	13	A	N3-C4-N9	7.92	133.74	127.40
22	BA	1689	A	C5-N7-C8	7.92	107.86	103.90
22	BA	1854	A	C4-C5-C6	7.92	120.96	117.00
23	BB	66	A	N3-C4-C5	-7.92	121.26	126.80
1	AA	435	A	C5-N7-C8	7.92	107.86	103.90
1	AA	1014	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2114	A	C4-C5-C6	7.92	120.96	117.00
1	AA	10	A	C8-N9-C4	7.92	108.97	105.80
22	BA	432	A	C5-N7-C8	7.92	107.86	103.90
22	BA	1700	A	C8-N9-C4	7.92	108.97	105.80
1	AA	205	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2471	A	C5-N7-C8	7.92	107.86	103.90
23	BB	29	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1821	A	N3-C4-C5	-7.91	121.26	126.80
1	AA	2	A	C5-N7-C8	7.91	107.86	103.90
1	AA	3	A	C5-N7-C8	7.91	107.85	103.90
1	AA	1102	A	N3-C4-N9	7.91	133.72	127.40
1	AA	190	A	C5-N7-C8	7.90	107.85	103.90
22	BA	1786	A	C5-N7-C8	7.90	107.85	103.90
22	BA	2052	A	N3-C4-N9	7.90	133.72	127.40
22	BA	2634	A	C5-N7-C8	7.90	107.85	103.90
1	AA	949	A	C5-N7-C8	7.90	107.85	103.90
1	AA	1483	A	C4-C5-C6	7.89	120.95	117.00
1	AA	1092	A	C5-N7-C8	7.89	107.85	103.90
22	BA	176	A	C5-C6-N6	7.89	130.01	123.70
22	BA	1322	A	C5-N7-C8	7.89	107.85	103.90
22	BA	575	A	C5-N7-C8	7.89	107.84	103.90
22	BA	1040	A	C5-N7-C8	7.89	107.84	103.90
22	BA	1785	A	N7-C8-N9	-7.89	109.86	113.80
22	BA	1981	A	C5-N7-C8	7.89	107.84	103.90
22	BA	2020	A	C5-N7-C8	7.89	107.84	103.90
22	BA	1054	A	N3-C4-N9	7.88	133.71	127.40
22	BA	1096	A	C5-N7-C8	7.88	107.84	103.90
1	AA	802	A	C8-N9-C4	7.88	108.95	105.80
22	BA	2765	A	N3-C4-N9	7.88	133.71	127.40
22	BA	207	A	N3-C4-C5	-7.88	121.28	126.80
22	BA	507	A	N7-C8-N9	-7.88	109.86	113.80
22	BA	743	A	N3-C4-N9	7.88	133.70	127.40
1	AA	441	A	C5-N7-C8	7.88	107.84	103.90
22	BA	644	A	N3-C4-N9	7.88	133.70	127.40
22	BA	2449	U	N3-C2-O2	-7.88	116.69	122.20
22	BA	2530	A	C5-N7-C8	7.88	107.84	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1016	A	C8-N9-C4	7.87	108.95	105.80
1	AA	996	A	C8-N9-C4	7.87	108.95	105.80
22	BA	2388	A	C4-C5-C6	7.87	120.93	117.00
1	AA	72	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1143	A	C4-C5-C6	7.86	120.93	117.00
22	BA	1553	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1981	A	N3-C4-C5	-7.86	121.30	126.80
22	BA	2309	A	C5-N7-C8	7.86	107.83	103.90
1	AA	373	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1739	A	N7-C8-N9	-7.86	109.87	113.80
22	BA	2776	A	C5-N7-C8	7.86	107.83	103.90
22	BA	382	A	C5-N7-C8	7.86	107.83	103.90
22	BA	983	A	C5-N7-C8	7.86	107.83	103.90
1	AA	353	A	C5-N7-C8	7.86	107.83	103.90
22	BA	556	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1434	A	C8-N9-C4	7.86	108.94	105.80
22	BA	2820	A	N3-C4-C5	-7.86	121.30	126.80
1	AA	179	A	C5-N7-C8	7.86	107.83	103.90
1	AA	1433	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2267	A	N3-C4-N9	7.86	133.69	127.40
1	AA	143	A	C5-N7-C8	7.85	107.83	103.90
22	BA	155	A	C5-N7-C8	7.85	107.83	103.90
1	AA	448	A	C5-N7-C8	7.85	107.83	103.90
1	AA	983	A	C5-N7-C8	7.85	107.82	103.90
1	AA	1005	A	C5-N7-C8	7.85	107.83	103.90
1	AA	706	A	C5-N7-C8	7.85	107.82	103.90
1	AA	1046	A	C5-N7-C8	7.85	107.82	103.90
22	BA	1156	A	N3-C4-N9	7.85	133.68	127.40
22	BA	1701	A	C5-N7-C8	7.85	107.82	103.90
22	BA	2060	A	C5-N7-C8	7.85	107.82	103.90
22	BA	1021	A	N3-C4-N9	7.84	133.68	127.40
22	BA	2560	A	C4-C5-C6	7.84	120.92	117.00
22	BA	213	A	C5-N7-C8	7.84	107.82	103.90
22	BA	789	A	N3-C4-N9	7.84	133.67	127.40
1	AA	1110	A	C5-N7-C8	7.83	107.82	103.90
22	BA	844	A	C5-N7-C8	7.83	107.81	103.90
22	BA	2679	A	C5-N7-C8	7.83	107.81	103.90
22	BA	685	A	N3-C4-N9	7.83	133.66	127.40
55	B8	51	A	C5-N7-C8	7.83	107.81	103.90
22	BA	226	A	C5-N7-C8	7.82	107.81	103.90
22	BA	1039	A	C5-N7-C8	7.82	107.81	103.90
22	BA	586	A	C5-N7-C8	7.82	107.81	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	743	A	C5-C6-N1	7.82	121.61	117.70
22	BA	1213	A	C8-N9-C4	7.82	108.93	105.80
22	BA	1287	A	N3-C4-N9	7.82	133.65	127.40
22	BA	1780	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2670	A	C8-N9-C4	7.82	108.93	105.80
1	AA	579	A	C5-N7-C8	7.81	107.81	103.90
1	AA	535	A	C8-N9-C4	7.81	108.92	105.80
1	AA	1021	A	N9-C4-C5	7.81	108.92	105.80
1	AA	1447	A	C5-N7-C8	7.81	107.81	103.90
22	BA	750	A	N3-C4-N9	7.81	133.65	127.40
22	BA	1668	A	N9-C4-C5	7.81	108.92	105.80
22	BA	1403	A	C5-N7-C8	7.81	107.80	103.90
22	BA	1977	A	C5-N7-C8	7.81	107.80	103.90
22	BA	2750	A	N3-C4-C5	-7.81	121.33	126.80
22	BA	892	A	C5-N7-C8	7.81	107.80	103.90
22	BA	1269	A	C4-C5-C6	7.81	120.90	117.00
22	BA	1801	A	C4-C5-C6	7.81	120.90	117.00
22	BA	2679	A	C5-C6-N1	7.81	121.60	117.70
1	AA	1000	A	C5-N7-C8	7.80	107.80	103.90
1	AA	1035	A	C5-N7-C8	7.80	107.80	103.90
1	AA	26	A	C5-N7-C8	7.80	107.80	103.90
22	BA	1254	A	C4-C5-C6	7.80	120.90	117.00
22	BA	2134	A	C5-N7-C8	7.80	107.80	103.90
1	AA	1329	A	C8-N9-C4	7.80	108.92	105.80
22	BA	2369	A	C5-N7-C8	7.80	107.80	103.90
22	BA	429	A	C5-N7-C8	7.80	107.80	103.90
22	BA	819	A	C5-N7-C8	7.80	107.80	103.90
22	BA	1302	A	N3-C4-C5	-7.80	121.34	126.80
22	BA	1598	A	C5-N7-C8	7.80	107.80	103.90
22	BA	2587	A	C4-C5-C6	7.80	120.90	117.00
1	AA	65	A	C5-N7-C8	7.80	107.80	103.90
1	AA	729	A	C5-N7-C8	7.80	107.80	103.90
1	AA	676	A	C5-N7-C8	7.80	107.80	103.90
1	AA	642	A	C5-N7-C8	7.79	107.80	103.90
22	BA	73	A	C5-N7-C8	7.79	107.80	103.90
1	AA	901	A	C5-N7-C8	7.79	107.80	103.90
22	BA	227	A	C5-N7-C8	7.79	107.80	103.90
22	BA	2003	A	C5-N7-C8	7.79	107.80	103.90
1	AA	320	A	C5-N7-C8	7.79	107.79	103.90
1	AA	1145	A	C5-N7-C8	7.79	107.79	103.90
22	BA	742	A	N3-C4-N9	7.79	133.63	127.40
23	BB	119	A	C5-N7-C8	7.79	107.79	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	681	A	C5-N7-C8	7.78	107.79	103.90
22	BA	1745	A	C5-N7-C8	7.78	107.79	103.90
22	BA	226	A	C4-C5-C6	7.78	120.89	117.00
22	BA	2015	A	C5-N7-C8	7.78	107.79	103.90
22	BA	344	A	C8-N9-C4	7.78	108.91	105.80
1	AA	306	A	C5-N7-C8	7.78	107.79	103.90
1	AA	1022	A	C5-N7-C8	7.78	107.79	103.90
22	BA	513	A	N3-C4-N9	7.78	133.62	127.40
22	BA	572	A	N3-C4-N9	7.77	133.62	127.40
22	BA	1287	A	C5-N7-C8	7.77	107.79	103.90
22	BA	251	A	N3-C4-N9	7.77	133.62	127.40
22	BA	2058	A	C5-N7-C8	7.77	107.79	103.90
22	BA	144	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1359	A	N9-C4-C5	7.77	108.91	105.80
22	BA	1532	A	C5-N7-C8	7.77	107.79	103.90
1	AA	336	A	N9-C4-C5	7.77	108.91	105.80
1	AA	994	A	C8-N9-C4	7.77	108.91	105.80
51	B3	32	ILE	CG1-CB-CG2	-7.77	94.31	111.40
1	AA	1151	A	C5-N7-C8	7.77	107.78	103.90
22	BA	613	A	C5-N7-C8	7.77	107.78	103.90
22	BA	705	A	C5-N7-C8	7.77	107.78	103.90
22	BA	1858	A	C5-N7-C8	7.77	107.78	103.90
22	BA	2114	A	N3-C4-N9	7.77	133.61	127.40
22	BA	508	A	C5-N7-C8	7.77	107.78	103.90
1	AA	1167	A	C5-N7-C8	7.76	107.78	103.90
22	BA	788	A	C8-N9-C4	7.76	108.91	105.80
22	BA	13	A	C5-N7-C8	7.76	107.78	103.90
22	BA	203	A	N3-C4-C5	-7.76	121.37	126.80
1	AA	499	A	C4-C5-C6	7.76	120.88	117.00
22	BA	826	U	OP2-P-O3'	-7.76	88.13	105.20
1	AA	983	A	C4-C5-C6	7.76	120.88	117.00
22	BA	928	A	C5-N7-C8	7.76	107.78	103.90
22	BA	621	A	N3-C4-C5	-7.75	121.37	126.80
22	BA	721	A	C5-N7-C8	7.75	107.78	103.90
55	B8	58	A	C5-N7-C8	7.75	107.78	103.90
1	AA	923	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1858	A	C8-N9-C4	7.75	108.90	105.80
22	BA	2281	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1655	A	C8-N9-C4	7.75	108.90	105.80
1	AA	906	A	C5-N7-C8	7.75	107.77	103.90
23	BB	119	A	C8-N9-C4	7.75	108.90	105.80
1	AA	451	A	C5-N7-C8	7.75	107.77	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	901	A	N3-C4-N9	7.75	133.60	127.40
22	BA	251	A	C5-N7-C8	7.75	107.77	103.90
22	BA	2199	A	C4-C5-C6	7.75	120.87	117.00
22	BA	528	A	C5-N7-C8	7.75	107.77	103.90
22	BA	973	A	N7-C8-N9	-7.75	109.93	113.80
1	AA	282	A	C5-N7-C8	7.74	107.77	103.90
22	BA	592	A	C5-N7-C8	7.74	107.77	103.90
22	BA	1336	A	C4-C5-C6	7.74	120.87	117.00
22	BA	1566	A	C5-N7-C8	7.74	107.77	103.90
22	BA	354	A	C5-N7-C8	7.74	107.77	103.90
1	AA	655	A	C5-N7-C8	7.74	107.77	103.90
22	BA	643	A	C5-N7-C8	7.74	107.77	103.90
22	BA	2657	A	C5-N7-C8	7.74	107.77	103.90
1	AA	456	A	C5-N7-C8	7.74	107.77	103.90
1	AA	1437	A	C5-N7-C8	7.74	107.77	103.90
22	BA	2497	A	C5-N7-C8	7.74	107.77	103.90
22	BA	1669	A	C4-C5-C6	7.74	120.87	117.00
1	AA	1150	A	C5-N7-C8	7.73	107.77	103.90
55	B8	26	A	C5-N7-C8	7.73	107.77	103.90
1	AA	1	A	C5-N7-C8	7.73	107.77	103.90
1	AA	411	A	C5-N7-C8	7.73	107.77	103.90
22	BA	794	A	C5-N7-C8	7.73	107.77	103.90
22	BA	1144	A	C5-N7-C8	7.73	107.77	103.90
22	BA	2434	A	C5-N7-C8	7.73	107.77	103.90
1	AA	320	A	C8-N9-C4	7.73	108.89	105.80
1	AA	914	A	C5-N7-C8	7.73	107.76	103.90
22	BA	1525	A	C5-N7-C8	7.73	107.76	103.90
22	BA	2635	A	C5-N7-C8	7.73	107.76	103.90
22	BA	332	A	C5-N7-C8	7.73	107.76	103.90
1	AA	1456	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1262	A	C5-N7-C8	7.72	107.76	103.90
22	BA	2407	A	C5-C6-N6	7.72	129.88	123.70
1	AA	1219	A	C5-C6-N6	7.72	129.88	123.70
1	AA	1362	A	C8-N9-C4	7.72	108.89	105.80
22	BA	471	A	C8-N9-C4	7.72	108.89	105.80
22	BA	2059	A	C8-N9-C4	7.72	108.89	105.80
1	AA	696	A	C4-C5-C6	7.72	120.86	117.00
1	AA	66	A	C5-C6-N6	7.72	129.87	123.70
1	AA	495	A	C8-N9-C4	7.72	108.89	105.80
22	BA	347	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1189	A	N3-C4-N9	7.72	133.57	127.40
22	BA	1608	A	N3-C4-N9	7.71	133.57	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2191	A	C5-N7-C8	7.71	107.76	103.90
1	AA	487	A	C5-N7-C8	7.71	107.76	103.90
22	BA	2451	A	N3-C4-C5	-7.71	121.40	126.80
1	AA	465	A	C5-N7-C8	7.71	107.75	103.90
1	AA	78	A	C8-N9-C4	7.71	108.88	105.80
22	BA	2388	A	N3-C4-N9	7.71	133.56	127.40
22	BA	460	A	C5-N7-C8	7.71	107.75	103.90
1	AA	60	A	C5-N7-C8	7.70	107.75	103.90
1	AA	608	A	C5-N7-C8	7.70	107.75	103.90
22	BA	925	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2564	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2660	A	C5-N7-C8	7.70	107.75	103.90
1	AA	1329	A	C5-N7-C8	7.70	107.75	103.90
22	BA	1552	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2062	A	C6-N1-C2	7.70	123.22	118.60
1	AA	560	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2015	A	C4-C5-C6	7.70	120.85	117.00
22	BA	981	A	C4-C5-C6	7.70	120.85	117.00
22	BA	1213	A	C5-C6-N6	7.70	129.86	123.70
22	BA	599	A	C5-N7-C8	7.69	107.75	103.90
22	BA	1032	A	C5-C6-N1	7.69	121.55	117.70
22	BA	1579	A	C5-N7-C8	7.69	107.75	103.90
22	BA	2147	A	C5-N7-C8	7.69	107.75	103.90
22	BA	492	A	C4-C5-C6	7.69	120.85	117.00
22	BA	2097	A	C4-C5-C6	7.69	120.85	117.00
1	AA	978	A	C5-N7-C8	7.69	107.74	103.90
22	BA	973	A	N9-C4-C5	7.69	108.88	105.80
22	BA	1419	A	C5-N7-C8	7.69	107.74	103.90
1	AA	1483	A	C5-N7-C8	7.69	107.74	103.90
22	BA	2176	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2639	A	C5-N7-C8	7.68	107.74	103.90
22	BA	643	A	C4-C5-C6	7.68	120.84	117.00
22	BA	677	A	C8-N9-C4	7.68	108.87	105.80
22	BA	443	A	C8-N9-C4	7.68	108.87	105.80
1	AA	675	A	C8-N9-C4	7.68	108.87	105.80
22	BA	127	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2886	A	C5-N7-C8	7.68	107.74	103.90
1	AA	452	A	C5-N7-C8	7.68	107.74	103.90
1	AA	728	A	C4-C5-C6	7.68	120.84	117.00
22	BA	501	A	C5-N7-C8	7.68	107.74	103.90
1	AA	510	A	C5-N7-C8	7.67	107.74	103.90
1	AA	873	A	C4-C5-C6	7.67	120.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	668	A	C8-N9-C4	7.67	108.87	105.80
22	BA	820	A	N3-C4-N9	7.67	133.54	127.40
22	BA	344	A	C5-N7-C8	7.67	107.73	103.90
22	BA	428	A	C5-N7-C8	7.67	107.73	103.90
22	BA	2352	A	C5-N7-C8	7.67	107.73	103.90
1	AA	51	A	C5-N7-C8	7.67	107.73	103.90
1	AA	171	A	C5-N7-C8	7.67	107.73	103.90
55	B8	38	A	C5-N7-C8	7.67	107.73	103.90
22	BA	42	A	C8-N9-C4	7.67	108.87	105.80
22	BA	1672	A	N3-C4-C5	-7.67	121.43	126.80
22	BA	1802	A	C4-C5-C6	7.67	120.83	117.00
1	AA	907	A	C4-C5-C6	7.66	120.83	117.00
1	AA	1170	A	C5-N7-C8	7.66	107.73	103.90
22	BA	146	A	C5-N7-C8	7.66	107.73	103.90
1	AA	151	A	C5-N7-C8	7.66	107.73	103.90
1	AA	706	A	C4-C5-C6	7.66	120.83	117.00
22	BA	447	A	C8-N9-C4	7.66	108.86	105.80
1	AA	182	A	C5-N7-C8	7.66	107.73	103.90
1	AA	1531	A	C5-N7-C8	7.66	107.73	103.90
1	AA	162	A	C5-N7-C8	7.65	107.73	103.90
22	BA	1784	A	C5-N7-C8	7.65	107.73	103.90
22	BA	2766	A	C5-C6-N1	7.65	121.53	117.70
1	AA	1339	A	C5-N7-C8	7.65	107.72	103.90
1	AA	313	A	C4-C5-C6	7.65	120.83	117.00
1	AA	629	A	C5-N7-C8	7.65	107.72	103.90
1	AA	873	A	C5-N7-C8	7.65	107.72	103.90
22	BA	196	A	N3-C4-N9	7.65	133.52	127.40
22	BA	1711	A	C8-N9-C4	7.65	108.86	105.80
22	BA	2850	A	C4-C5-C6	7.65	120.82	117.00
22	BA	2799	A	N3-C4-N9	7.65	133.52	127.40
22	BA	789	A	C5-N7-C8	7.64	107.72	103.90
1	AA	116	A	C8-N9-C4	7.64	108.86	105.80
22	BA	1477	A	C5-N7-C8	7.64	107.72	103.90
22	BA	1593	A	C8-N9-C4	7.64	108.86	105.80
1	AA	1495	U	N3-C2-O2	-7.64	116.85	122.20
22	BA	2412	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2534	A	C5-N7-C8	7.64	107.72	103.90
22	BA	256	A	C4-C5-C6	7.64	120.82	117.00
22	BA	2433	A	C4-C5-C6	7.64	120.82	117.00
1	AA	1188	A	C5-N7-C8	7.63	107.72	103.90
22	BA	637	A	C5-N7-C8	7.63	107.72	103.90
1	AA	461	A	N3-C4-C5	-7.63	121.46	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1241	A	C5-N7-C8	7.63	107.72	103.90
22	BA	2019	A	N3-C4-C5	-7.63	121.46	126.80
1	AA	1201	A	C8-N9-C4	7.63	108.85	105.80
22	BA	789	A	C8-N9-C4	7.63	108.85	105.80
22	BA	1090	A	C4-C5-C6	7.63	120.81	117.00
22	BA	1783	A	C8-N9-C4	7.63	108.85	105.80
1	AA	1176	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1287	A	C4-C5-C6	7.63	120.81	117.00
22	BA	2311	A	C5-N7-C8	7.63	107.71	103.90
1	AA	59	A	C5-N7-C8	7.62	107.71	103.90
1	AA	432	A	C5-N7-C8	7.62	107.71	103.90
1	AA	969	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1614	A	N3-C4-C5	-7.62	121.47	126.80
1	AA	493	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1705	A	C5-N7-C8	7.62	107.71	103.90
1	AA	80	A	C4-C5-C6	7.62	120.81	117.00
1	AA	574	A	C5-N7-C8	7.62	107.71	103.90
1	AA	766	A	C5-N7-C8	7.62	107.71	103.90
1	AA	1239	A	C8-N9-C4	7.62	108.85	105.80
22	BA	320	A	C8-N9-C4	7.62	108.85	105.80
22	BA	2614	A	N3-C4-N9	7.62	133.49	127.40
55	B8	42	A	C5-N7-C8	7.62	107.71	103.90
22	BA	502	A	N9-C4-C5	7.61	108.84	105.80
22	BA	2358	A	C8-N9-C4	7.61	108.84	105.80
22	BA	454	A	C5-N7-C8	7.61	107.71	103.90
22	BA	2700	A	C5-N7-C8	7.61	107.71	103.90
1	AA	181	A	C5-N7-C8	7.61	107.70	103.90
22	BA	676	A	N3-C4-C5	-7.61	121.47	126.80
22	BA	2719	G	N9-C4-C5	-7.61	102.36	105.40
22	BA	49	A	C5-N7-C8	7.61	107.70	103.90
22	BA	1156	A	C8-N9-C4	7.61	108.84	105.80
1	AA	327	A	C8-N9-C4	7.61	108.84	105.80
22	BA	1032	A	C8-N9-C4	7.61	108.84	105.80
22	BA	1353	A	C5-N7-C8	7.61	107.70	103.90
55	B8	76	A	C4-C5-N7	-7.61	106.90	110.70
1	AA	98	A	C5-N7-C8	7.61	107.70	103.90
22	BA	432	A	C8-N9-C4	7.61	108.84	105.80
22	BA	453	A	C5-N7-C8	7.61	107.70	103.90
22	BA	2288	A	C5-N7-C8	7.61	107.70	103.90
22	BA	1169	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1698	A	C5-N7-C8	7.60	107.70	103.90
22	BA	2059	A	C5-N7-C8	7.60	107.70	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	34	A	C8-N9-C4	7.60	108.84	105.80
23	BB	108	A	C5-N7-C8	7.60	107.70	103.90
1	AA	573	A	C5-N7-C8	7.60	107.70	103.90
1	AA	663	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1938	A	C4-C5-C6	7.60	120.80	117.00
22	BA	2813	A	C5-N7-C8	7.60	107.70	103.90
1	AA	608	A	C8-N9-C4	7.60	108.84	105.80
1	AA	1239	A	C5-N7-C8	7.60	107.70	103.90
1	AA	1363	A	C4-C5-C6	7.60	120.80	117.00
22	BA	1522	A	C5-N7-C8	7.60	107.70	103.90
22	BA	2453	A	C4-C5-C6	7.60	120.80	117.00
1	AA	482	A	C5-N7-C8	7.60	107.70	103.90
1	AA	116	A	C5-C6-N6	7.59	129.78	123.70
22	BA	742	A	C5-N7-C8	7.59	107.70	103.90
22	BA	892	A	OP1-P-OP2	-7.59	108.21	119.60
22	BA	1046	A	C5-N7-C8	7.59	107.70	103.90
22	BA	1608	A	C5-N7-C8	7.59	107.70	103.90
22	BA	2176	A	C4-C5-C6	7.59	120.80	117.00
22	BA	1275	A	C4-C5-C6	7.59	120.80	117.00
1	AA	1271	A	C5-N7-C8	7.59	107.69	103.90
22	BA	1365	A	N3-C4-N9	7.59	133.47	127.40
22	BA	2211	A	C8-N9-C4	7.59	108.84	105.80
22	BA	1054	A	C4-C5-C6	7.59	120.79	117.00
22	BA	1744	A	C5-N7-C8	7.59	107.69	103.90
1	AA	382	A	C5-N7-C8	7.58	107.69	103.90
1	AA	1236	A	N3-C4-N9	7.58	133.47	127.40
1	AA	1269	A	C5-N7-C8	7.58	107.69	103.90
22	BA	216	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2377	A	C4-C5-C6	7.58	120.79	117.00
1	AA	937	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1175	A	C5-N7-C8	7.58	107.69	103.90
1	AA	630	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1365	A	C5-N7-C8	7.58	107.69	103.90
1	AA	53	A	C5-N7-C8	7.58	107.69	103.90
1	AA	983	A	N3-C4-N9	7.58	133.46	127.40
22	BA	161	A	C5-N7-C8	7.58	107.69	103.90
22	BA	820	A	C4-C5-C6	7.57	120.79	117.00
55	B8	6	A	C5-N7-C8	7.57	107.69	103.90
1	AA	1468	A	C4-C5-C6	7.57	120.78	117.00
22	BA	1009	A	N3-C4-N9	7.57	133.46	127.40
1	AA	1055	A	C5-N7-C8	7.57	107.68	103.90
1	AA	393	A	C8-N9-C4	7.57	108.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	532	A	C5-N7-C8	7.57	107.68	103.90
1	AA	1082	A	C5-N7-C8	7.57	107.68	103.90
22	BA	2600	A	C5-N7-C8	7.57	107.68	103.90
22	BA	2733	A	C5-N7-C8	7.57	107.68	103.90
54	B7	9	A	C4-C5-C6	7.57	120.78	117.00
22	BA	1156	A	C5-N7-C8	7.56	107.68	103.90
1	AA	695	A	C5-N7-C8	7.56	107.68	103.90
1	AA	1236	A	C5-N7-C8	7.56	107.68	103.90
22	BA	2278	A	C5-N7-C8	7.56	107.68	103.90
55	B8	21	A	C5-N7-C8	7.56	107.68	103.90
1	AA	68	G	C5-N7-C8	-7.56	100.52	104.30
22	BA	689	A	C5-C6-N6	7.56	129.75	123.70
22	BA	616	A	C4-C5-C6	7.56	120.78	117.00
22	BA	1773	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1978	A	C5-N7-C8	7.56	107.68	103.90
22	BA	2541	A	C5-N7-C8	7.56	107.68	103.90
55	B8	41	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1213	A	C4-C5-C6	7.55	120.78	117.00
22	BA	2799	A	C5-C6-N6	7.55	129.74	123.70
22	BA	783	A	C5-N7-C8	7.55	107.68	103.90
22	BA	900	A	C8-N9-C4	7.55	108.82	105.80
22	BA	1342	A	C5-N7-C8	7.55	107.68	103.90
22	BA	1936	A	N3-C4-N9	7.55	133.44	127.40
22	BA	2198	A	C5-N7-C8	7.55	107.67	103.90
22	BA	176	A	C5-N7-C8	7.55	107.67	103.90
22	BA	2577	A	C4-C5-C6	7.55	120.78	117.00
1	AA	958	A	C5-N7-C8	7.55	107.67	103.90
22	BA	716	A	C5-N7-C8	7.55	107.67	103.90
22	BA	1590	A	C5-N7-C8	7.55	107.67	103.90
22	BA	2565	A	C8-N9-C4	7.55	108.82	105.80
22	BA	2766	A	N3-C4-N9	7.55	133.44	127.40
1	AA	635	A	C5-N7-C8	7.54	107.67	103.90
1	AA	1171	A	C4-C5-C6	7.54	120.77	117.00
23	BB	78	A	C5-N7-C8	7.54	107.67	103.90
55	B8	76	A	C5-N7-C8	7.54	107.67	103.90
22	BA	899	A	C5-N7-C8	7.54	107.67	103.90
1	AA	197	A	C5-N7-C8	7.54	107.67	103.90
1	AA	535	A	C5-N7-C8	7.54	107.67	103.90
1	AA	546	A	C5-N7-C8	7.54	107.67	103.90
22	BA	155	A	C4-C5-C6	7.54	120.77	117.00
22	BA	529	A	C4-C5-N7	-7.54	106.93	110.70
1	AA	889	A	N9-C4-C5	7.54	108.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	909	A	C5-N7-C8	7.54	107.67	103.90
22	BA	1395	A	C5-N7-C8	7.54	107.67	103.90
22	BA	2451	A	N9-C4-C5	7.54	108.81	105.80
22	BA	2518	A	N3-C4-N9	7.54	133.43	127.40
22	BA	1359	A	C5-N7-C8	7.53	107.67	103.90
22	BA	2451	A	N7-C8-N9	-7.53	110.03	113.80
1	AA	915	A	C5-N7-C8	7.53	107.67	103.90
22	BA	1204	A	N9-C4-C5	7.53	108.81	105.80
22	BA	1802	A	C5-C6-N6	7.53	129.72	123.70
22	BA	2675	A	C8-N9-C4	7.53	108.81	105.80
1	AA	607	A	C5-N7-C8	7.53	107.67	103.90
22	BA	1938	A	N3-C4-N9	7.53	133.42	127.40
1	AA	746	A	C5-N7-C8	7.53	107.66	103.90
22	BA	19	A	C4-C5-C6	7.53	120.76	117.00
22	BA	734	A	C5-N7-C8	7.53	107.66	103.90
22	BA	505	A	C8-N9-C4	7.52	108.81	105.80
1	AA	1046	A	N3-C4-N9	7.52	133.42	127.40
1	AA	199	A	C4-C5-C6	7.52	120.76	117.00
22	BA	676	A	C5-N7-C8	7.52	107.66	103.90
1	AA	303	A	C5-N7-C8	7.52	107.66	103.90
1	AA	949	A	C4-C5-C6	7.52	120.76	117.00
22	BA	2439	A	C8-N9-C4	7.51	108.81	105.80
22	BA	975	A	C8-N9-C4	7.51	108.81	105.80
1	AA	1171	A	N3-C4-N9	7.51	133.41	127.40
22	BA	1913	A	C5-N7-C8	7.51	107.65	103.90
22	BA	2425	A	C4-C5-C6	7.51	120.75	117.00
22	BA	979	A	C8-N9-C4	7.51	108.80	105.80
22	BA	471	A	N3-C4-N9	7.50	133.40	127.40
22	BA	1419	A	C5-C6-N1	7.50	121.45	117.70
22	BA	160	A	C5-N7-C8	7.50	107.65	103.90
22	BA	599	A	C5-C6-N1	7.50	121.45	117.70
22	BA	1384	A	C5-N7-C8	7.50	107.65	103.90
1	AA	1225	A	C5-N7-C8	7.50	107.65	103.90
1	AA	1357	A	C5-N7-C8	7.50	107.65	103.90
1	AA	1507	A	C5-N7-C8	7.50	107.65	103.90
22	BA	761	A	C4-C5-C6	7.50	120.75	117.00
22	BA	1508	A	C8-N9-C4	7.50	108.80	105.80
1	AA	1163	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2094	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2736	A	C5-N7-C8	7.50	107.65	103.90
1	AA	228	A	C8-N9-C4	7.50	108.80	105.80
22	BA	470	A	C4-C5-C6	7.50	120.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	579	A	C8-N9-C4	7.49	108.80	105.80
22	BA	2411	A	C5-N7-C8	7.49	107.65	103.90
1	AA	374	A	C5-N7-C8	7.49	107.65	103.90
22	BA	2450	A	C8-N9-C4	7.49	108.80	105.80
22	BA	74	A	C5-N7-C8	7.49	107.64	103.90
22	BA	453	A	C8-N9-C4	7.49	108.80	105.80
1	AA	1102	A	C4-C5-C6	7.48	120.74	117.00
22	BA	2753	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2448	A	C4-C5-C6	7.48	120.74	117.00
22	BA	2711	A	C5-C6-N1	7.48	121.44	117.70
22	BA	2800	A	N9-C4-C5	7.48	108.79	105.80
55	B8	59	A	C5-N7-C8	7.48	107.64	103.90
1	AA	559	A	C4-C5-C6	7.48	120.74	117.00
1	AA	1169	A	C5-N7-C8	7.48	107.64	103.90
22	BA	14	A	C5-N7-C8	7.48	107.64	103.90
22	BA	412	A	C4-C5-C6	7.48	120.74	117.00
22	BA	2726	A	C8-N9-C4	7.48	108.79	105.80
23	BB	52	A	C5-N7-C8	7.48	107.64	103.90
1	AA	98	A	C5-C6-N6	7.48	129.68	123.70
22	BA	352	A	C8-N9-C4	7.47	108.79	105.80
22	BA	2388	A	C8-N9-C4	7.47	108.79	105.80
23	BB	57	A	C4-C5-C6	7.47	120.74	117.00
22	BA	483	A	C5-N7-C8	7.47	107.64	103.90
22	BA	1213	A	C5-N7-C8	7.47	107.64	103.90
22	BA	1678	A	C4-C5-C6	7.47	120.73	117.00
22	BA	1780	A	C4-C5-C6	7.47	120.73	117.00
1	AA	55	A	C4-C5-C6	7.47	120.73	117.00
1	AA	338	A	C5-N7-C8	7.47	107.63	103.90
22	BA	2860	A	C5-N7-C8	7.47	107.63	103.90
1	AA	1261	A	C4-C5-C6	7.47	120.73	117.00
22	BA	827	U	O5'-P-OP1	7.47	119.66	110.70
22	BA	2077	A	C4-C5-C6	7.46	120.73	117.00
1	AA	353	A	C8-N9-C4	7.46	108.78	105.80
1	AA	814	A	C4-C5-C6	7.46	120.73	117.00
1	AA	1196	A	C5-N7-C8	7.46	107.63	103.90
22	BA	362	A	C4-C5-C6	7.46	120.73	117.00
22	BA	513	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1048	A	C5-N7-C8	7.46	107.63	103.90
22	BA	181	A	C5-N7-C8	7.46	107.63	103.90
1	AA	572	A	C8-N9-C4	7.46	108.78	105.80
22	BA	165	A	C5-N7-C8	7.46	107.63	103.90
22	BA	348	A	C5-N7-C8	7.46	107.63	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	504	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1086	A	N9-C4-C5	7.46	108.78	105.80
22	BA	1757	A	N3-C4-C5	-7.46	121.58	126.80
1	AA	77	A	C8-N9-C4	7.46	108.78	105.80
22	BA	470	A	C5-N7-C8	7.46	107.63	103.90
1	AA	435	A	C8-N9-C4	7.45	108.78	105.80
22	BA	677	A	N3-C4-N9	7.45	133.36	127.40
22	BA	1054	A	C5-N7-C8	7.45	107.63	103.90
22	BA	2288	A	N3-C4-N9	7.45	133.36	127.40
22	BA	1815	A	C5-N7-C8	7.45	107.63	103.90
22	BA	1854	A	C5-N7-C8	7.45	107.62	103.90
22	BA	1039	A	C8-N9-C4	7.45	108.78	105.80
22	BA	1572	A	N3-C4-N9	7.45	133.36	127.40
22	BA	2095	A	C5-N7-C8	7.45	107.62	103.90
1	AA	430	A	N3-C4-N9	7.45	133.36	127.40
22	BA	1001	A	C5-N7-C8	7.45	107.62	103.90
22	BA	2453	A	N9-C4-C5	7.45	108.78	105.80
22	BA	980	A	C4-C5-C6	7.44	120.72	117.00
1	AA	816	A	C5-N7-C8	7.44	107.62	103.90
1	AA	32	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1689	A	C4-C5-C6	7.44	120.72	117.00
1	AA	397	A	N3-C4-N9	7.44	133.35	127.40
22	BA	621	A	C8-N9-C4	7.44	108.78	105.80
1	AA	80	A	C5-N7-C8	7.44	107.62	103.90
1	AA	520	A	N9-C4-C5	7.44	108.78	105.80
22	BA	2461	A	N3-C4-N9	7.44	133.35	127.40
22	BA	1809	A	C4-C5-C6	7.44	120.72	117.00
1	AA	33	A	C5-N7-C8	7.43	107.62	103.90
1	AA	533	A	N3-C4-N9	7.43	133.35	127.40
22	BA	299	A	C5-N7-C8	7.43	107.62	103.90
22	BA	2212	A	C5-N7-C8	7.43	107.62	103.90
22	BA	2566	A	N3-C4-C5	-7.43	121.60	126.80
1	AA	174	A	C4-C5-C6	7.43	120.72	117.00
22	BA	348	A	C8-N9-C4	7.43	108.77	105.80
22	BA	781	A	C4-C5-C6	7.43	120.71	117.00
22	BA	538	A	C8-N9-C4	7.43	108.77	105.80
22	BA	825	A	N9-C4-C5	7.43	108.77	105.80
22	BA	2432	A	C8-N9-C4	7.43	108.77	105.80
22	BA	1815	A	C8-N9-C4	7.42	108.77	105.80
22	BA	2665	A	C8-N9-C4	7.42	108.77	105.80
1	AA	1254	A	C5-N7-C8	7.42	107.61	103.90
22	BA	231	A	C4-C5-C6	7.42	120.71	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	960	A	C4-C5-C6	7.42	120.71	117.00
22	BA	1088	A	C5-N7-C8	7.42	107.61	103.90
22	BA	2531	A	C4-C5-C6	7.42	120.71	117.00
1	AA	412	A	C5-N7-C8	7.42	107.61	103.90
22	BA	458	G	O4'-C1'-N9	7.42	114.14	108.20
1	AA	1534	A	C4-C5-C6	7.42	120.71	117.00
1	AA	900	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1204	A	C4-C5-N7	-7.42	106.99	110.70
1	AA	553	A	C5-N7-C8	7.42	107.61	103.90
1	AA	1046	A	C4-C5-C6	7.41	120.71	117.00
22	BA	1354	A	C8-N9-C4	7.41	108.77	105.80
22	BA	1373	A	N3-C4-N9	7.41	133.33	127.40
1	AA	130	A	C5-N7-C8	7.41	107.61	103.90
1	AA	16	A	C5-N7-C8	7.41	107.61	103.90
1	AA	336	A	C5-N7-C8	7.41	107.61	103.90
1	AA	414	A	C8-N9-C4	7.41	108.76	105.80
22	BA	176	A	C8-N9-C4	7.41	108.76	105.80
22	BA	1528	A	N3-C4-N9	7.41	133.33	127.40
22	BA	1754	A	C4-C5-C6	7.41	120.70	117.00
22	BA	1759	A	C5-N7-C8	7.41	107.60	103.90
22	BA	2434	A	C5-C6-N1	7.41	121.40	117.70
23	BB	46	A	C5-N7-C8	7.41	107.60	103.90
1	AA	1431	A	C5-N7-C8	7.41	107.60	103.90
22	BA	675	A	C5-C6-N6	7.41	129.62	123.70
1	AA	802	A	N3-C4-N9	7.40	133.32	127.40
22	BA	2077	A	N3-C4-N9	7.40	133.32	127.40
22	BA	2835	A	C5-N7-C8	7.40	107.60	103.90
1	AA	329	A	C4-C5-C6	7.40	120.70	117.00
22	BA	1847	A	C4-C5-C6	7.40	120.70	117.00
1	AA	975	A	C5-N7-C8	7.40	107.60	103.90
22	BA	2335	A	C8-N9-C4	7.40	108.76	105.80
22	BA	1090	A	N3-C4-N9	7.40	133.32	127.40
1	AA	915	A	N3-C4-C5	-7.39	121.62	126.80
22	BA	1080	A	C5-N7-C8	7.39	107.60	103.90
22	BA	1549	A	C5-N7-C8	7.39	107.60	103.90
1	AA	195	A	C5-N7-C8	7.39	107.60	103.90
22	BA	85	G	O5'-P-OP2	-7.39	99.05	105.70
22	BA	2386	A	C4-C5-C6	7.39	120.70	117.00
22	BA	631	A	C8-N9-C4	7.39	108.76	105.80
22	BA	279	A	C4-C5-C6	7.39	120.69	117.00
22	BA	1057	A	C5-N7-C8	7.39	107.59	103.90
22	BA	1580	A	C4-C5-C6	7.39	120.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1626	A	C8-N9-C4	7.39	108.75	105.80
22	BA	219	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2328	A	C4-C5-C6	7.38	120.69	117.00
1	AA	523	A	C5-N7-C8	7.38	107.59	103.90
1	AA	665	A	C5-N7-C8	7.38	107.59	103.90
22	BA	439	A	C5-C6-N1	7.38	121.39	117.70
22	BA	1890	A	C5-N7-C8	7.38	107.59	103.90
1	AA	1101	A	C8-N9-C4	7.38	108.75	105.80
22	BA	1871	A	C5-N7-C8	7.38	107.59	103.90
1	AA	780	A	C5-N7-C8	7.38	107.59	103.90
1	AA	1324	A	C5-N7-C8	7.38	107.59	103.90
22	BA	743	A	C5-N7-C8	7.38	107.59	103.90
22	BA	1027	A	C5-N7-C8	7.38	107.59	103.90
22	BA	1194	A	C8-N9-C4	7.38	108.75	105.80
22	BA	1431	A	C5-N7-C8	7.38	107.59	103.90
1	AA	366	A	C5-N7-C8	7.37	107.59	103.90
1	AA	431	A	C5-N7-C8	7.37	107.59	103.90
1	AA	1105	A	C8-N9-C4	7.37	108.75	105.80
22	BA	1610	A	C5-N7-C8	7.37	107.59	103.90
22	BA	195	A	N7-C8-N9	-7.37	110.11	113.80
22	BA	1535	A	C5-N7-C8	7.37	107.58	103.90
22	BA	2459	A	N3-C4-N9	7.37	133.30	127.40
1	AA	1021	A	C4-C5-N7	-7.37	107.02	110.70
22	BA	861	A	C5-N7-C8	7.37	107.58	103.90
22	BA	927	A	C5-N7-C8	7.37	107.58	103.90
22	BA	1086	A	C5-N7-C8	7.37	107.58	103.90
22	BA	730	A	C5-N7-C8	7.36	107.58	103.90
22	BA	677	A	C5-C6-N6	7.36	129.59	123.70
1	AA	865	A	C4-C5-C6	7.36	120.68	117.00
22	BA	2381	A	C5-N7-C8	7.36	107.58	103.90
22	BA	2412	A	C8-N9-C4	7.36	108.74	105.80
1	AA	109	A	C5-N7-C8	7.36	107.58	103.90
22	BA	2614	A	N9-C4-C5	7.36	108.74	105.80
22	BA	1246	A	C4-C5-C6	7.35	120.68	117.00
22	BA	2566	A	C8-N9-C4	7.35	108.74	105.80
22	BA	2589	A	C5-C6-N1	7.35	121.38	117.70
22	BA	310	A	C5-N7-C8	7.35	107.57	103.90
22	BA	19	A	N3-C4-N9	7.35	133.28	127.40
22	BA	1090	A	C5-N7-C8	7.35	107.57	103.90
22	BA	2101	A	C5-N7-C8	7.35	107.57	103.90
22	BA	1854	A	C8-N9-C4	7.34	108.74	105.80
1	AA	365	U	C5-C4-O4	7.34	130.31	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	936	A	C5-N7-C8	7.34	107.57	103.90
55	B8	66	A	C5-N7-C8	7.34	107.57	103.90
1	AA	1117	A	C5-N7-C8	7.34	107.57	103.90
1	AA	1418	A	N3-C4-N9	7.34	133.27	127.40
22	BA	1434	A	C5-N7-C8	7.34	107.57	103.90
1	AA	19	A	N9-C4-C5	7.33	108.73	105.80
22	BA	1630	A	N9-C4-C5	7.33	108.73	105.80
22	BA	2142	A	C5-N7-C8	7.33	107.56	103.90
1	AA	223	A	C5-N7-C8	7.33	107.56	103.90
1	AA	300	A	N3-C4-N9	7.33	133.26	127.40
1	AA	878	A	C5-N7-C8	7.33	107.56	103.90
1	AA	1080	A	C4-C5-C6	7.33	120.66	117.00
1	AA	356	A	N3-C4-N9	7.33	133.26	127.40
22	BA	300	A	C5-N7-C8	7.33	107.56	103.90
22	BA	1067	A	C5-N7-C8	7.33	107.56	103.90
22	BA	2565	A	N3-C4-N9	7.33	133.26	127.40
22	BA	505	A	C4-C5-C6	7.32	120.66	117.00
22	BA	1304	A	C5-N7-C8	7.32	107.56	103.90
22	BA	2090	A	C5-C6-N1	7.32	121.36	117.70
22	BA	945	A	N9-C4-C5	7.32	108.73	105.80
1	AA	1213	A	C8-N9-C4	7.32	108.73	105.80
1	AA	1250	A	C5-N7-C8	7.32	107.56	103.90
22	BA	2183	A	C5-N7-C8	7.32	107.56	103.90
1	AA	889	A	C5-N7-C8	7.32	107.56	103.90
22	BA	514	A	C5-N7-C8	7.32	107.56	103.90
22	BA	1165	A	C8-N9-C4	7.32	108.73	105.80
22	BA	1144	A	N3-C4-N9	7.31	133.25	127.40
22	BA	2497	A	N9-C4-C5	7.31	108.73	105.80
22	BA	781	A	C5-N7-C8	7.31	107.56	103.90
22	BA	1077	A	C5-N7-C8	7.31	107.56	103.90
22	BA	1794	A	C5-N7-C8	7.31	107.56	103.90
1	AA	1196	A	C8-N9-C4	7.31	108.72	105.80
22	BA	320	A	C5-N7-C8	7.31	107.56	103.90
22	BA	63	A	C8-N9-C4	7.31	108.72	105.80
22	BA	342	A	C5-N7-C8	7.31	107.55	103.90
22	BA	1354	A	N3-C4-N9	7.31	133.25	127.40
22	BA	155	A	N3-C4-N9	7.31	133.25	127.40
22	BA	802	A	C4-C5-C6	7.30	120.65	117.00
1	AA	32	A	N3-C4-N9	7.30	133.24	127.40
22	BA	1439	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1872	A	N3-C4-N9	7.30	133.24	127.40
1	AA	1288	A	C5-N7-C8	7.30	107.55	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	983	A	N3-C4-N9	7.30	133.24	127.40
22	BA	2602	A	C4-C5-N7	-7.30	107.05	110.70
22	BA	2799	A	C8-N9-C4	7.30	108.72	105.80
22	BA	2377	A	N3-C4-N9	7.30	133.24	127.40
22	BA	2764	A	N9-C4-C5	7.30	108.72	105.80
22	BA	2482	A	C8-N9-C4	7.30	108.72	105.80
22	BA	1787	A	C5-N7-C8	7.29	107.55	103.90
22	BA	167	A	C4-C5-C6	7.29	120.65	117.00
22	BA	602	A	C8-N9-C4	7.29	108.72	105.80
22	BA	1634	A	C8-N9-C4	7.29	108.72	105.80
22	BA	2899	A	C5-C6-N6	7.29	129.53	123.70
23	BB	46	A	C4-C5-C6	7.29	120.65	117.00
22	BA	1029	A	C5-N7-C8	7.29	107.55	103.90
1	AA	794	A	C5-N7-C8	7.29	107.54	103.90
22	BA	503	A	N3-C4-N9	7.29	133.23	127.40
22	BA	1981	A	C8-N9-C4	7.29	108.72	105.80
1	AA	80	A	N3-C4-N9	7.29	133.23	127.40
22	BA	845	A	C5-C6-N1	7.29	121.34	117.70
1	AA	609	A	C4-C5-C6	7.28	120.64	117.00
1	AA	1434	A	C5-N7-C8	7.28	107.54	103.90
22	BA	152	A	C5-N7-C8	7.28	107.54	103.90
22	BA	899	A	C8-N9-C4	7.28	108.71	105.80
22	BA	1336	A	N3-C4-N9	7.28	133.23	127.40
22	BA	95	A	C5-N7-C8	7.28	107.54	103.90
22	BA	309	A	N3-C4-N9	7.28	133.22	127.40
22	BA	2459	A	C5-N7-C8	7.28	107.54	103.90
22	BA	2560	A	C5-N7-C8	7.28	107.54	103.90
22	BA	572	A	C5-N7-C8	7.28	107.54	103.90
22	BA	1383	A	C5-N7-C8	7.28	107.54	103.90
22	BA	1705	A	N3-C4-N9	7.28	133.22	127.40
22	BA	1746	A	C5-N7-C8	7.28	107.54	103.90
1	AA	766	A	C8-N9-C4	7.28	108.71	105.80
1	AA	1332	A	C4-C5-C6	7.28	120.64	117.00
22	BA	56	A	C5-N7-C8	7.28	107.54	103.90
22	BA	794	A	C5-C6-N1	7.28	121.34	117.70
22	BA	1427	A	N3-C4-C5	-7.28	121.71	126.80
1	AA	1019	A	C5-N7-C8	7.28	107.54	103.90
1	AA	1349	A	C5-N7-C8	7.28	107.54	103.90
22	BA	2792	A	C4-C5-C6	7.28	120.64	117.00
22	BA	1269	A	N3-C4-N9	7.27	133.22	127.40
22	BA	1899	A	C5-N7-C8	7.27	107.54	103.90
1	AA	53	A	C4-C5-C6	7.27	120.64	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1080	A	C5-N7-C8	7.27	107.54	103.90
22	BA	654	A	N3-C4-N9	7.27	133.22	127.40
22	BA	1302	A	C8-N9-C4	7.27	108.71	105.80
1	AA	1346	A	C8-N9-C4	7.27	108.71	105.80
1	AA	1483	A	N3-C4-N9	7.27	133.22	127.40
22	BA	1810	A	C5-C6-N6	7.27	129.52	123.70
22	BA	2097	A	C5-N7-C8	7.27	107.53	103.90
22	BA	2577	A	N3-C4-N9	7.27	133.22	127.40
22	BA	793	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1591	A	N3-C4-N9	7.27	133.21	127.40
1	AA	807	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1134	A	N3-C4-N9	7.26	133.21	127.40
1	AA	510	A	C8-N9-C4	7.26	108.70	105.80
1	AA	1093	A	C5-N7-C8	7.26	107.53	103.90
1	AA	768	A	C4-C5-C6	7.26	120.63	117.00
22	BA	231	A	N3-C4-N9	7.26	133.21	127.40
1	AA	1289	A	C5-N7-C8	7.26	107.53	103.90
22	BA	627	A	C4-C5-C6	7.26	120.63	117.00
22	BA	2765	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1953	A	C4-C5-C6	7.25	120.63	117.00
1	AA	747	A	C5-N7-C8	7.25	107.53	103.90
1	AA	946	A	C5-N7-C8	7.25	107.53	103.90
1	AA	1468	A	N3-C4-N9	7.25	133.20	127.40
22	BA	2886	A	C8-N9-C4	7.25	108.70	105.80
22	BA	764	A	C5-N7-C8	7.25	107.52	103.90
22	BA	2184	A	C4-C5-C6	7.25	120.62	117.00
1	AA	161	A	C5-N7-C8	7.25	107.52	103.90
1	AA	1170	A	C4-C5-C6	7.25	120.62	117.00
22	BA	800	A	C5-N7-C8	7.25	107.52	103.90
23	BB	57	A	C5-N7-C8	7.25	107.52	103.90
1	AA	906	A	N3-C4-N9	7.24	133.19	127.40
1	AA	1261	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1133	A	C4-C5-N7	-7.24	107.08	110.70
22	BA	1952	A	C5-N7-C8	7.24	107.52	103.90
22	BA	2899	A	C5-N7-C8	7.24	107.52	103.90
1	AA	1238	A	C4-C5-C6	7.24	120.62	117.00
22	BA	751	A	C4-C5-C6	7.24	120.62	117.00
1	AA	907	A	N3-C4-N9	7.24	133.19	127.40
22	BA	1987	A	N3-C4-N9	7.24	133.19	127.40
22	BA	602	A	C5-N7-C8	7.24	107.52	103.90
22	BA	2340	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1591	A	C5-C6-N1	7.23	121.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2205	A	C4-C5-C6	7.23	120.62	117.00
1	AA	356	A	C8-N9-C4	7.23	108.69	105.80
1	AA	1046	A	C8-N9-C4	7.23	108.69	105.80
22	BA	1572	A	C5-C6-N6	7.23	129.49	123.70
1	AA	974	A	C8-N9-C4	7.23	108.69	105.80
22	BA	402	A	C5-N7-C8	7.23	107.51	103.90
22	BA	449	A	N3-C4-N9	7.23	133.18	127.40
22	BA	1080	A	N9-C4-C5	7.23	108.69	105.80
22	BA	1143	A	N3-C4-N9	7.23	133.18	127.40
22	BA	2461	A	C4-C5-C6	7.23	120.61	117.00
1	AA	715	A	C8-N9-C4	7.23	108.69	105.80
22	BA	2037	A	C5-N7-C8	7.23	107.51	103.90
1	AA	19	A	C4-C5-C6	7.22	120.61	117.00
22	BA	1609	A	N3-C4-N9	7.22	133.18	127.40
1	AA	60	A	N9-C4-C5	7.22	108.69	105.80
22	BA	1009	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1722	A	C4-C5-C6	7.22	120.61	117.00
22	BA	477	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1773	A	N3-C4-N9	7.22	133.18	127.40
22	BA	1365	A	C4-C5-C6	7.22	120.61	117.00
1	AA	1236	A	C4-C5-C6	7.22	120.61	117.00
22	BA	2268	A	C4-C5-C6	7.22	120.61	117.00
22	BA	2602	A	N9-C4-C5	7.22	108.69	105.80
1	AA	1081	A	C8-N9-C4	7.21	108.69	105.80
1	AA	1502	A	C4-C5-C6	7.21	120.61	117.00
22	BA	988	A	C5-N7-C8	7.21	107.51	103.90
22	BA	2097	A	N3-C4-N9	7.21	133.17	127.40
22	BA	2386	A	C8-N9-C4	7.21	108.69	105.80
22	BA	2721	A	C4-C5-C6	7.21	120.61	117.00
22	BA	2764	A	C5-C6-N1	7.21	121.31	117.70
22	BA	2821	A	N3-C4-N9	7.21	133.17	127.40
1	AA	1256	A	C4-C5-C6	7.21	120.61	117.00
22	BA	2366	A	C4-C5-C6	7.21	120.61	117.00
22	BA	1302	A	C5-N7-C8	7.21	107.50	103.90
22	BA	2005	A	C5-N7-C8	7.21	107.50	103.90
1	AA	243	A	N9-C4-C5	7.21	108.68	105.80
22	BA	63	A	C5-N7-C8	7.21	107.50	103.90
22	BA	1089	A	C5-N7-C8	7.21	107.50	103.90
22	BA	401	A	C4-C5-C6	7.21	120.60	117.00
22	BA	471	A	C4-C5-C6	7.21	120.60	117.00
22	BA	909	A	C5-C6-N1	7.21	121.30	117.70
22	BA	1810	A	C5-N7-C8	7.21	107.50	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1705	A	C5-C6-N1	7.21	121.30	117.70
22	BA	2679	A	C4-C5-C6	7.21	120.60	117.00
1	AA	1082	A	C4-C5-C6	7.20	120.60	117.00
22	BA	563	A	C8-N9-C4	7.20	108.68	105.80
22	BA	1970	A	N3-C4-N9	7.20	133.16	127.40
22	BA	196	A	C4-C5-C6	7.20	120.60	117.00
22	BA	845	A	N3-C4-N9	7.20	133.16	127.40
22	BA	2090	A	N3-C4-N9	7.20	133.16	127.40
1	AA	935	A	C8-N9-C4	7.20	108.68	105.80
1	AA	1306	A	C8-N9-C4	7.20	108.68	105.80
22	BA	1735	A	C5-N7-C8	7.20	107.50	103.90
22	BA	2899	A	C4-C5-C6	7.20	120.60	117.00
1	AA	673	A	N3-C4-N9	7.20	133.16	127.40
22	BA	2468	A	C5-N7-C8	7.20	107.50	103.90
22	BA	844	A	C8-N9-C4	7.20	108.68	105.80
1	AA	716	A	C5-N7-C8	7.19	107.50	103.90
22	BA	2792	A	N3-C4-N9	7.19	133.16	127.40
1	AA	356	A	C4-C5-C6	7.19	120.60	117.00
1	AA	415	A	C5-N7-C8	7.19	107.50	103.90
22	BA	56	A	N3-C4-N9	7.19	133.15	127.40
55	B8	69	A	C5-N7-C8	7.19	107.50	103.90
22	BA	1603	A	C5-N7-C8	7.19	107.49	103.90
22	BA	2101	A	C4-C5-C6	7.19	120.59	117.00
1	AA	329	A	N3-C4-N9	7.18	133.15	127.40
22	BA	19	A	C5-N7-C8	7.18	107.49	103.90
1	AA	460	A	C5-N7-C8	7.18	107.49	103.90
1	AA	914	A	C4-C5-C6	7.18	120.59	117.00
1	AA	1287	A	C5-N7-C8	7.18	107.49	103.90
22	BA	689	A	N3-C4-N9	7.18	133.15	127.40
22	BA	1596	A	C8-N9-C4	7.18	108.67	105.80
22	BA	1664	A	C5-N7-C8	7.18	107.49	103.90
23	BB	104	A	C5-N7-C8	7.18	107.49	103.90
1	AA	298	A	C5-N7-C8	7.18	107.49	103.90
1	AA	1238	A	C5-N7-C8	7.18	107.49	103.90
1	AA	1507	A	N9-C4-C5	7.18	108.67	105.80
22	BA	330	A	N3-C4-N9	7.18	133.14	127.40
22	BA	131	A	C8-N9-C4	7.18	108.67	105.80
22	BA	384	A	C5-N7-C8	7.18	107.49	103.90
1	AA	715	A	C5-N7-C8	7.17	107.49	103.90
22	BA	1571	A	C4-C5-C6	7.17	120.59	117.00
22	BA	1877	A	C5-N7-C8	7.17	107.49	103.90
22	BA	2052	A	C4-C5-C6	7.17	120.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	994	A	N3-C4-N9	7.17	133.14	127.40
22	BA	1819	A	C4-C5-C6	7.17	120.59	117.00
22	BA	1853	A	C5-N7-C8	7.17	107.48	103.90
23	BB	101	A	C4-C5-N7	-7.17	107.11	110.70
1	AA	120	A	C5-N7-C8	7.17	107.48	103.90
1	AA	1229	A	C5-N7-C8	7.17	107.48	103.90
22	BA	2547	A	C5-N7-C8	7.17	107.48	103.90
1	AA	814	A	N3-C4-N9	7.17	133.13	127.40
1	AA	913	A	C5-N7-C8	7.17	107.48	103.90
22	BA	368	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1378	A	C8-N9-C4	7.17	108.67	105.80
22	BA	590	A	C5-N7-C8	7.16	107.48	103.90
22	BA	1819	A	N3-C4-N9	7.16	133.13	127.40
1	AA	1163	A	C8-N9-C4	7.16	108.66	105.80
1	AA	1508	A	C5-N7-C8	7.16	107.48	103.90
22	BA	1	G	OP1-P-OP2	-7.16	108.86	119.60
22	BA	1000	A	N3-C4-N9	7.16	133.13	127.40
22	BA	1286	A	C5-N7-C8	7.16	107.48	103.90
22	BA	1759	A	N3-C4-N9	7.16	133.13	127.40
22	BA	1027	A	N3-C4-C5	-7.16	121.79	126.80
22	BA	1809	A	C5-N7-C8	7.16	107.48	103.90
1	AA	878	A	C8-N9-C4	7.15	108.66	105.80
1	AA	1408	A	C8-N9-C4	7.15	108.66	105.80
22	BA	1809	A	N3-C4-N9	7.15	133.12	127.40
1	AA	389	A	C4-C5-C6	7.15	120.58	117.00
22	BA	255	A	C4-C5-C6	7.15	120.58	117.00
1	AA	573	A	C4-C5-C6	7.15	120.58	117.00
22	BA	244	A	C5-N7-C8	7.15	107.47	103.90
22	BA	1932	A	C5-N7-C8	7.15	107.47	103.90
22	BA	2757	A	N3-C4-N9	7.15	133.12	127.40
1	AA	908	A	C5-N7-C8	7.15	107.47	103.90
1	AA	1146	A	C5-N7-C8	7.15	107.47	103.90
22	BA	340	A	C4-C5-C6	7.15	120.57	117.00
22	BA	685	A	C5-N7-C8	7.15	107.47	103.90
1	AA	262	A	C5-N7-C8	7.14	107.47	103.90
1	AA	964	A	C5-N7-C8	7.14	107.47	103.90
22	BA	689	A	C5-C6-N1	7.14	121.27	117.70
22	BA	1470	A	C5-N7-C8	7.14	107.47	103.90
22	BA	2062	A	C5-N7-C8	7.14	107.47	103.90
23	BB	73	A	C8-N9-C4	7.14	108.66	105.80
1	AA	908	A	N3-C4-N9	7.14	133.11	127.40
22	BA	362	A	N3-C4-N9	7.14	133.11	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1268	A	C5-N7-C8	7.14	107.47	103.90
22	BA	1502	A	C5-N7-C8	7.14	107.47	103.90
1	AA	190	A	N3-C4-N9	7.14	133.11	127.40
22	BA	2893	A	C4-C5-C6	7.14	120.57	117.00
1	AA	1216	A	C5-N7-C8	7.13	107.47	103.90
22	BA	1133	A	C4-C5-C6	7.13	120.57	117.00
22	BA	2469	A	C8-N9-C4	7.13	108.65	105.80
1	AA	49	U	N3-C4-O4	-7.13	114.41	119.40
1	AA	706	A	N3-C4-N9	7.13	133.11	127.40
22	BA	911	A	C4-C5-C6	7.13	120.57	117.00
22	BA	1230	A	C5-N7-C8	7.13	107.47	103.90
1	AA	196	A	C5-N7-C8	7.13	107.46	103.90
1	AA	366	A	C4-C5-C6	7.13	120.56	117.00
1	AA	482	A	C8-N9-C4	7.13	108.65	105.80
1	AA	1179	A	N9-C4-C5	7.13	108.65	105.80
22	BA	1552	A	C4-C5-C6	7.13	120.56	117.00
22	BA	1805	A	C8-N9-C4	7.13	108.65	105.80
22	BA	2247	A	C5-N7-C8	7.13	107.46	103.90
22	BA	2439	A	C5-N7-C8	7.13	107.46	103.90
22	BA	2560	A	N3-C4-N9	7.12	133.10	127.40
1	AA	1167	A	C8-N9-C4	7.12	108.65	105.80
1	AA	321	A	C8-N9-C4	7.12	108.65	105.80
22	BA	191	A	C4-C5-C6	7.12	120.56	117.00
22	BA	715	A	C5-N7-C8	7.12	107.46	103.90
22	BA	1847	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2614	A	C4-C5-N7	-7.12	107.14	110.70
22	BA	616	A	N3-C4-N9	7.12	133.09	127.40
22	BA	2799	A	C4-C5-C6	7.12	120.56	117.00
1	AA	938	A	N3-C4-N9	7.11	133.09	127.40
1	AA	1151	A	C8-N9-C4	7.11	108.64	105.80
22	BA	1127	A	C5-N7-C8	7.11	107.46	103.90
22	BA	1387	A	N3-C4-N9	7.11	133.09	127.40
22	BA	2733	A	C8-N9-C4	7.11	108.64	105.80
22	BA	497	A	C5-N7-C8	7.11	107.45	103.90
22	BA	1373	A	C5-N7-C8	7.11	107.45	103.90
1	AA	794	A	C8-N9-C4	7.11	108.64	105.80
1	AA	1152	A	N3-C4-N9	7.11	133.09	127.40
1	AA	1252	A	C5-N7-C8	7.10	107.45	103.90
1	AA	397	A	C5-N7-C8	7.10	107.45	103.90
1	AA	655	A	C4-C5-C6	7.10	120.55	117.00
1	AA	712	A	C8-N9-C4	7.10	108.64	105.80
1	AA	1508	A	C4-C5-C6	7.10	120.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1569	A	C5-N7-C8	7.10	107.45	103.90
1	AA	802	A	C4-C5-C6	7.10	120.55	117.00
22	BA	1802	A	N3-C4-N9	7.10	133.08	127.40
22	BA	233	A	C8-N9-C4	7.09	108.64	105.80
22	BA	1254	A	N3-C4-N9	7.09	133.07	127.40
22	BA	2170	A	C5-N7-C8	7.09	107.45	103.90
22	BA	2820	A	C5-N7-C8	7.09	107.44	103.90
22	BA	751	A	C5-N7-C8	7.09	107.44	103.90
22	BA	910	A	C5-N7-C8	7.09	107.44	103.90
1	AA	1396	A	N3-C4-N9	7.08	133.07	127.40
22	BA	2406	A	C5-N7-C8	7.08	107.44	103.90
1	AA	520	A	C4-C5-N7	-7.08	107.16	110.70
22	BA	2449	U	N3-C4-C5	7.08	118.85	114.60
22	BA	2851	A	C5-N7-C8	7.08	107.44	103.90
1	AA	415	A	C4-C5-C6	7.08	120.54	117.00
1	AA	487	A	C4-C5-C6	7.08	120.54	117.00
1	AA	784	A	C4-C5-C6	7.08	120.54	117.00
22	BA	1328	A	C5-N7-C8	7.08	107.44	103.90
1	AA	609	A	C5-N7-C8	7.08	107.44	103.90
22	BA	2134	A	C8-N9-C4	7.08	108.63	105.80
22	BA	2247	A	C8-N9-C4	7.08	108.63	105.80
1	AA	167	A	N3-C4-N9	7.07	133.06	127.40
22	BA	64	A	N3-C4-N9	7.07	133.06	127.40
22	BA	1690	A	C4-C5-C6	7.07	120.54	117.00
1	AA	338	A	N3-C4-N9	7.07	133.06	127.40
1	AA	397	A	C4-C5-C6	7.07	120.54	117.00
1	AA	1219	A	N3-C4-N9	7.07	133.06	127.40
22	BA	1151	A	C5-N7-C8	7.07	107.44	103.90
1	AA	583	A	C4-C5-N7	-7.07	107.16	110.70
1	AA	781	A	N3-C4-N9	7.07	133.06	127.40
22	BA	1494	A	C5-N7-C8	7.07	107.43	103.90
1	AA	546	A	N3-C4-N9	7.07	133.05	127.40
22	BA	94	A	C5-N7-C8	7.07	107.43	103.90
22	BA	819	A	N3-C4-N9	7.06	133.05	127.40
22	BA	845	A	C8-N9-C4	7.06	108.62	105.80
22	BA	1553	A	C4-C5-C6	7.06	120.53	117.00
22	BA	2191	A	C4-C5-C6	7.06	120.53	117.00
1	AA	373	A	C8-N9-C4	7.06	108.62	105.80
22	BA	213	A	C5-C6-N1	7.06	121.23	117.70
1	AA	1468	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1189	A	C4-C5-C6	7.06	120.53	117.00
22	BA	1272	A	C5-N7-C8	7.06	107.43	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2381	A	C8-N9-C4	7.06	108.62	105.80
22	BA	608	A	C8-N9-C4	7.06	108.62	105.80
22	BA	800	A	N3-C4-C5	-7.05	121.86	126.80
1	AA	665	A	C8-N9-C4	7.05	108.62	105.80
22	BA	2108	A	C4-C5-C6	7.05	120.53	117.00
1	AA	1044	A	C5-N7-C8	7.05	107.42	103.90
22	BA	173	A	C8-N9-C4	7.05	108.62	105.80
1	AA	152	A	C8-N9-C4	7.05	108.62	105.80
1	AA	749	A	C5-N7-C8	7.05	107.42	103.90
22	BA	632	A	C5-N7-C8	7.05	107.42	103.90
22	BA	1678	A	C8-N9-C4	7.05	108.62	105.80
22	BA	2135	A	C5-N7-C8	7.05	107.42	103.90
22	BA	1722	A	C8-N9-C4	7.04	108.62	105.80
22	BA	753	A	N3-C4-N9	7.04	133.03	127.40
23	BB	109	A	N3-C4-N9	7.04	133.03	127.40
22	BA	265	A	C8-N9-C4	7.04	108.62	105.80
22	BA	2358	A	C5-N7-C8	7.04	107.42	103.90
22	BA	2706	A	C5-N7-C8	7.04	107.42	103.90
22	BA	270	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1304	A	N9-C4-C5	7.04	108.62	105.80
1	AA	44	A	C4-C5-C6	7.04	120.52	117.00
1	AA	363	A	N3-C4-N9	7.04	133.03	127.40
23	BB	109	A	C4-C5-C6	7.04	120.52	117.00
22	BA	915	C	C6-N1-C2	-7.04	117.48	120.30
22	BA	2059	A	C5-C6-N6	7.04	129.33	123.70
22	BA	422	A	N3-C4-N9	7.03	133.03	127.40
22	BA	927	A	C8-N9-C4	7.03	108.61	105.80
22	BA	2322	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2776	A	C8-N9-C4	7.03	108.61	105.80
1	AA	1394	A	C5-N7-C8	7.03	107.41	103.90
22	BA	706	A	C4-C5-C6	7.03	120.51	117.00
1	AA	1067	A	C8-N9-C4	7.03	108.61	105.80
22	BA	1808	A	C5-N7-C8	7.03	107.41	103.90
22	BA	2340	A	N3-C4-N9	7.03	133.02	127.40
22	BA	632	A	C4-C5-C6	7.02	120.51	117.00
1	AA	329	A	C5-N7-C8	7.02	107.41	103.90
1	AA	1275	A	C8-N9-C4	7.02	108.61	105.80
1	AA	1340	A	C8-N9-C4	7.02	108.61	105.80
22	BA	586	A	C8-N9-C4	7.02	108.61	105.80
22	BA	722	A	C5-C6-N1	7.02	121.21	117.70
23	BB	58	A	C4-C5-C6	7.02	120.51	117.00
1	AA	1225	A	N3-C4-N9	7.02	133.01	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1	A	N3-C4-N9	7.01	133.01	127.40
22	BA	401	A	N3-C4-N9	7.01	133.01	127.40
22	BA	514	A	C8-N9-C4	7.01	108.61	105.80
22	BA	1654	A	C5-N7-C8	7.01	107.41	103.90
22	BA	1762	A	N9-C4-C5	7.01	108.61	105.80
1	AA	167	A	C4-C5-C6	7.01	120.50	117.00
22	BA	2810	A	C8-N9-C4	7.01	108.60	105.80
1	AA	162	A	N3-C4-N9	7.01	133.01	127.40
1	AA	1507	A	C4-C5-C6	7.01	120.50	117.00
22	BA	483	A	C4-C5-C6	7.00	120.50	117.00
22	BA	849	A	C4-C5-C6	7.00	120.50	117.00
22	BA	1490	A	N3-C4-N9	7.00	133.00	127.40
1	AA	815	A	C4-C5-C6	7.00	120.50	117.00
1	AA	906	A	C4-C5-C6	7.00	120.50	117.00
22	BA	282	A	C8-N9-C4	7.00	108.60	105.80
22	BA	878	A	C8-N9-C4	7.00	108.60	105.80
22	BA	1913	A	C4-C5-C6	7.00	120.50	117.00
22	BA	2450	A	N3-C4-N9	7.00	133.00	127.40
1	AA	363	A	C4-C5-C6	7.00	120.50	117.00
22	BA	2764	A	C5-N7-C8	7.00	107.40	103.90
22	BA	2778	A	C4-C5-C6	7.00	120.50	117.00
22	BA	447	A	C4-C5-C6	7.00	120.50	117.00
22	BA	1669	A	N3-C4-N9	7.00	133.00	127.40
22	BA	1613	G	N1-C6-O6	-7.00	115.70	119.90
1	AA	975	A	C4-C5-C6	6.99	120.50	117.00
22	BA	1508	A	C4-C5-C6	6.99	120.50	117.00
1	AA	353	A	C4-C5-C6	6.99	120.50	117.00
22	BA	722	A	N3-C4-N9	6.99	132.99	127.40
22	BA	2142	A	C4-C5-C6	6.99	120.50	117.00
23	BB	29	A	C4-C5-C6	6.99	120.50	117.00
22	BA	2407	A	C4-C5-C6	6.99	120.50	117.00
1	AA	1152	A	C4-C5-C6	6.99	120.49	117.00
22	BA	223	A	C5-N7-C8	6.99	107.39	103.90
22	BA	829	A	C4-C5-C6	6.99	120.49	117.00
22	BA	1583	A	C8-N9-C4	6.99	108.59	105.80
22	BA	2635	A	C5-C6-N1	6.99	121.19	117.70
22	BA	190	A	C4-C5-C6	6.99	120.49	117.00
22	BA	1419	A	C8-N9-C4	6.99	108.59	105.80
22	BA	1580	A	C8-N9-C4	6.99	108.59	105.80
22	BA	2530	A	C8-N9-C4	6.99	108.59	105.80
22	BA	1635	A	C5-N7-C8	6.98	107.39	103.90
22	BA	176	A	C5-C6-N1	6.98	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1301	A	N3-C4-N9	6.98	132.99	127.40
22	BA	2298	A	C8-N9-C4	6.98	108.59	105.80
22	BA	91	A	C5-N7-C8	6.98	107.39	103.90
22	BA	203	A	C8-N9-C4	6.98	108.59	105.80
22	BA	1885	A	C4-C5-C6	6.98	120.49	117.00
22	BA	2298	A	C5-N7-C8	6.98	107.39	103.90
22	BA	2814	A	C5-N7-C8	6.98	107.39	103.90
1	AA	499	A	N3-C4-N9	6.98	132.98	127.40
1	AA	622	A	C5-N7-C8	6.98	107.39	103.90
22	BA	960	A	C4-C5-N7	-6.98	107.21	110.70
22	BA	1509	A	C8-N9-C4	6.97	108.59	105.80
22	BA	2741	A	C5-N7-C8	6.97	107.39	103.90
22	BA	981	A	C5-N7-C8	6.97	107.39	103.90
1	AA	130	A	N3-C4-N9	6.97	132.98	127.40
1	AA	1465	A	C8-N9-C4	6.97	108.59	105.80
22	BA	2052	A	C5-C6-N1	6.97	121.19	117.70
22	BA	2317	A	C4-C5-C6	6.97	120.48	117.00
22	BA	270	A	C8-N9-C4	6.97	108.59	105.80
22	BA	1142	A	C4-C5-C6	6.96	120.48	117.00
1	AA	461	A	C5-N7-C8	6.96	107.38	103.90
1	AA	968	A	C4-C5-C6	6.96	120.48	117.00
22	BA	2108	A	C5-N7-C8	6.96	107.38	103.90
1	AA	100	G	C5-C6-O6	-6.96	124.42	128.60
1	AA	1274	A	C5-N7-C8	6.96	107.38	103.90
22	BA	975	A	N3-C4-N9	6.96	132.97	127.40
22	BA	1301	A	C4-C5-C6	6.96	120.48	117.00
22	BA	2054	A	C4-C5-C6	6.96	120.48	117.00
22	BA	2660	A	C4-C5-C6	6.96	120.48	117.00
1	AA	69	G	C2-N3-C4	6.96	115.38	111.90
1	AA	1280	A	C8-N9-C4	6.96	108.58	105.80
22	BA	1205	A	C5-N7-C8	6.96	107.38	103.90
22	BA	1226	A	C4-C5-C6	6.96	120.48	117.00
1	AA	1375	A	C4-C5-C6	6.96	120.48	117.00
22	BA	1073	A	C4-C5-C6	6.96	120.48	117.00
1	AA	1130	A	C5-N7-C8	6.95	107.38	103.90
22	BA	1609	A	C4-C5-C6	6.95	120.48	117.00
1	AA	743	A	C5-N7-C8	6.95	107.38	103.90
1	AA	780	A	C4-C5-C6	6.95	120.47	117.00
22	BA	655	A	C4-C5-C6	6.95	120.48	117.00
22	BA	699	A	C4-C5-C6	6.95	120.48	117.00
1	AA	456	A	C8-N9-C4	6.95	108.58	105.80
22	BA	131	A	N3-C4-N9	6.95	132.96	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1126	A	C5-N7-C8	6.95	107.37	103.90
22	BA	1705	A	C8-N9-C4	6.95	108.58	105.80
1	AA	55	A	N3-C4-N9	6.95	132.96	127.40
1	AA	1299	A	C5-N7-C8	6.95	107.37	103.90
1	AA	563	A	N9-C4-C5	6.95	108.58	105.80
22	BA	42	A	C5-N7-C8	6.95	107.37	103.90
22	BA	190	A	N3-C4-N9	6.94	132.96	127.40
22	BA	226	A	N3-C4-N9	6.94	132.95	127.40
22	BA	1274	A	C4-C5-C6	6.94	120.47	117.00
1	AA	432	A	C4-C5-C6	6.94	120.47	117.00
22	BA	233	A	C5-N7-C8	6.94	107.37	103.90
1	AA	374	A	N3-C4-N9	6.94	132.95	127.40
22	BA	1470	A	C8-N9-C4	6.94	108.58	105.80
22	BA	1593	A	C5-N7-C8	6.94	107.37	103.90
1	AA	199	A	C5-N7-C8	6.93	107.37	103.90
22	BA	1901	A	N3-C4-N9	6.93	132.95	127.40
22	BA	2662	A	C5-N7-C8	6.93	107.37	103.90
22	BA	1276	A	N3-C4-N9	6.93	132.95	127.40
22	BA	1470	A	C4-C5-C6	6.93	120.47	117.00
22	BA	391	A	N3-C4-N9	6.93	132.94	127.40
22	BA	401	A	C8-N9-C4	6.93	108.57	105.80
1	AA	456	A	N3-C4-N9	6.93	132.94	127.40
1	AA	1111	A	C4-C5-C6	6.93	120.47	117.00
1	AA	702	A	C4-C5-C6	6.93	120.46	117.00
1	AA	1219	A	C4-C5-C6	6.93	120.46	117.00
22	BA	2051	A	N3-C4-N9	6.93	132.94	127.40
23	BB	94	A	N3-C4-N9	6.93	132.94	127.40
22	BA	2199	A	N3-C4-N9	6.92	132.94	127.40
1	AA	160	A	N9-C4-C5	6.92	108.57	105.80
22	BA	2335	A	C4-C5-N7	-6.92	107.24	110.70
22	BA	309	A	C8-N9-C4	6.92	108.57	105.80
22	BA	2590	A	C5-N7-C8	6.92	107.36	103.90
1	AA	300	A	C5-N7-C8	6.92	107.36	103.90
22	BA	980	A	N3-C4-N9	6.92	132.93	127.40
22	BA	2336	A	C5-N7-C8	6.92	107.36	103.90
22	BA	2433	A	C8-N9-C4	6.92	108.57	105.80
22	BA	1439	A	C4-C5-C6	6.92	120.46	117.00
22	BA	2119	A	N9-C4-C5	6.92	108.57	105.80
22	BA	2433	A	N3-C4-N9	6.92	132.93	127.40
23	BB	109	A	C5-N7-C8	6.92	107.36	103.90
22	BA	95	A	C4-C5-C6	6.91	120.46	117.00
1	AA	197	A	C8-N9-C4	6.91	108.56	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	583	A	C4-C5-C6	6.91	120.46	117.00
22	BA	626	A	C8-N9-C4	6.91	108.56	105.80
22	BA	1134	A	C4-C5-C6	6.91	120.46	117.00
22	BA	1274	A	N3-C4-N9	6.91	132.93	127.40
22	BA	1545	A	C5-N7-C8	6.91	107.36	103.90
22	BA	1735	A	N3-C4-N9	6.91	132.93	127.40
1	AA	792	A	N3-C4-N9	6.91	132.93	127.40
22	BA	91	A	C8-N9-C4	6.91	108.56	105.80
1	AA	389	A	N3-C4-N9	6.91	132.93	127.40
22	BA	586	A	C4-C5-C6	6.91	120.45	117.00
1	AA	493	A	C8-N9-C4	6.91	108.56	105.80
1	AA	1225	A	C4-C5-C6	6.91	120.45	117.00
22	BA	231	A	C5-C6-N1	6.91	121.15	117.70
22	BA	1434	A	C4-C5-C6	6.91	120.45	117.00
22	BA	2432	A	C4-C5-C6	6.91	120.45	117.00
1	AA	1257	A	C8-N9-C4	6.90	108.56	105.80
22	BA	423	A	C5-N7-C8	6.90	107.35	103.90
22	BA	793	A	C4-C5-C6	6.90	120.45	117.00
22	BA	1528	A	C8-N9-C4	6.90	108.56	105.80
22	BA	1609	A	C8-N9-C4	6.90	108.56	105.80
22	BA	2284	A	N3-C4-N9	6.90	132.92	127.40
23	BB	94	A	C4-C5-C6	6.90	120.45	117.00
1	AA	282	A	C8-N9-C4	6.90	108.56	105.80
1	AA	1256	A	C8-N9-C4	6.90	108.56	105.80
1	AA	1456	A	C8-N9-C4	6.90	108.56	105.80
22	BA	2377	A	C5-N7-C8	6.90	107.35	103.90
22	BA	2090	A	C8-N9-C4	6.90	108.56	105.80
1	AA	199	A	N3-C4-N9	6.90	132.92	127.40
22	BA	2077	A	C8-N9-C4	6.90	108.56	105.80
22	BA	1284	A	C5-N7-C8	6.90	107.35	103.90
22	BA	1936	A	C5-N7-C8	6.90	107.35	103.90
22	BA	91	A	C4-C5-C6	6.89	120.45	117.00
22	BA	2799	A	C5-N7-C8	6.89	107.35	103.90
1	AA	1350	A	C4-C5-C6	6.89	120.45	117.00
22	BA	167	A	C8-N9-C4	6.89	108.56	105.80
22	BA	195	A	C5-C6-N1	6.89	121.15	117.70
22	BA	654	A	C5-N7-C8	6.89	107.35	103.90
22	BA	793	A	N3-C4-N9	6.89	132.91	127.40
22	BA	1021	A	C4-C5-N7	-6.89	107.25	110.70
22	BA	1241	A	N3-C4-N9	6.89	132.91	127.40
23	BB	109	A	C8-N9-C4	6.89	108.56	105.80
22	BA	83	A	C8-N9-C4	6.89	108.56	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1253	A	C5-C6-N1	6.89	121.15	117.70
22	BA	1998	A	N9-C4-C5	6.89	108.56	105.80
1	AA	487	A	N3-C4-N9	6.89	132.91	127.40
22	BA	127	A	C4-C5-C6	6.89	120.44	117.00
22	BA	1630	A	C4-C5-N7	-6.89	107.25	110.70
22	BA	1690	A	N9-C4-C5	6.89	108.56	105.80
1	AA	573	A	C8-N9-C4	6.89	108.56	105.80
22	BA	255	A	C8-N9-C4	6.88	108.55	105.80
22	BA	1572	A	C8-N9-C4	6.88	108.55	105.80
22	BA	2184	A	C5-N7-C8	6.88	107.34	103.90
1	AA	554	A	N9-C4-C5	6.88	108.55	105.80
22	BA	2900	A	C5-N7-C8	6.88	107.34	103.90
23	BB	115	A	C8-N9-C4	6.88	108.55	105.80
1	AA	452	A	C8-N9-C4	6.88	108.55	105.80
1	AA	523	A	C4-C5-C6	6.88	120.44	117.00
22	BA	299	A	N9-C4-C5	6.88	108.55	105.80
22	BA	761	A	N3-C4-N9	6.88	132.91	127.40
22	BA	927	A	N3-C4-N9	6.88	132.91	127.40
22	BA	1848	A	N7-C8-N9	-6.88	110.36	113.80
22	BA	2813	A	C4-C5-C6	6.88	120.44	117.00
23	BB	39	A	C5-N7-C8	6.88	107.34	103.90
22	BA	541	A	C4-C5-C6	6.88	120.44	117.00
1	AA	781	A	C4-C5-C6	6.88	120.44	117.00
1	AA	1368	A	C8-N9-C4	6.88	108.55	105.80
22	BA	1590	A	N3-C4-N9	6.88	132.90	127.40
22	BA	960	A	N9-C4-C5	6.88	108.55	105.80
22	BA	1048	A	N3-C4-N9	6.88	132.90	127.40
22	BA	2602	A	C8-N9-C4	6.88	108.55	105.80
22	BA	1247	A	C5-C6-N1	6.87	121.14	117.70
1	AA	321	A	N3-C4-N9	6.87	132.90	127.40
1	AA	1261	A	N3-C4-N9	6.87	132.90	127.40
22	BA	1549	A	N3-C4-N9	6.87	132.90	127.40
22	BA	71	A	C8-N9-C4	6.87	108.55	105.80
22	BA	677	A	C4-C5-C6	6.87	120.43	117.00
22	BA	1596	A	C4-C5-C6	6.87	120.43	117.00
22	BA	1791	A	C4-C5-C6	6.87	120.44	117.00
22	BA	2766	A	C8-N9-C4	6.87	108.55	105.80
1	AA	1067	A	C4-C5-C6	6.87	120.43	117.00
22	BA	751	A	N3-C4-N9	6.87	132.89	127.40
22	BA	1757	A	C5-N7-C8	6.87	107.33	103.90
22	BA	2095	A	C4-C5-C6	6.87	120.43	117.00
22	BA	2899	A	N3-C4-N9	6.87	132.89	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	347	A	N9-C4-C5	6.86	108.55	105.80
22	BA	503	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1960	A	C5-C6-N1	6.86	121.13	117.70
22	BA	2792	A	C5-N7-C8	6.86	107.33	103.90
22	BA	996	A	C5-N7-C8	6.86	107.33	103.90
22	BA	705	A	N3-C4-N9	6.86	132.89	127.40
22	BA	1103	A	C5-N7-C8	6.86	107.33	103.90
22	BA	1469	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1640	A	N9-C4-C5	6.86	108.54	105.80
22	BA	2868	A	C5-N7-C8	6.86	107.33	103.90
22	BA	1572	A	C5-N7-C8	6.86	107.33	103.90
22	BA	666	A	C4-C5-C6	6.85	120.43	117.00
1	AA	279	A	C4-C5-C6	6.85	120.43	117.00
1	AA	1377	A	C8-N9-C4	6.85	108.54	105.80
22	BA	2662	A	N9-C4-C5	6.85	108.54	105.80
22	BA	382	A	C4-C5-C6	6.85	120.43	117.00
22	BA	2476	A	C5-N7-C8	6.85	107.33	103.90
55	B8	69	A	N3-C4-N9	6.85	132.88	127.40
22	BA	2020	A	C8-N9-C4	6.85	108.54	105.80
1	AA	718	A	C5-N7-C8	6.85	107.32	103.90
22	BA	1490	A	C4-C5-C6	6.85	120.42	117.00
22	BA	1927	A	C5-N7-C8	6.85	107.32	103.90
1	AA	1339	A	C4-C5-C6	6.85	120.42	117.00
22	BA	980	A	C5-N7-C8	6.85	107.32	103.90
22	BA	1260	A	C8-N9-C4	6.84	108.54	105.80
22	BA	1413	A	C5-N7-C8	6.84	107.32	103.90
1	AA	274	A	C8-N9-C4	6.84	108.54	105.80
1	AA	964	A	C4-C5-C6	6.84	120.42	117.00
1	AA	1480	A	C8-N9-C4	6.84	108.54	105.80
1	AA	1483	A	C8-N9-C4	6.84	108.54	105.80
22	BA	1969	A	C5-N7-C8	6.84	107.32	103.90
1	AA	949	A	N3-C4-N9	6.84	132.87	127.40
22	BA	10	A	C5-N7-C8	6.84	107.32	103.90
22	BA	28	A	C4-C5-C6	6.84	120.42	117.00
22	BA	1328	A	N9-C4-C5	6.84	108.53	105.80
22	BA	279	A	C5-N7-C8	6.84	107.32	103.90
22	BA	300	A	C4-C5-C6	6.84	120.42	117.00
22	BA	1387	A	C4-C5-C6	6.84	120.42	117.00
1	AA	694	A	N3-C4-N9	6.83	132.87	127.40
22	BA	104	A	C5-N7-C8	6.83	107.32	103.90
22	BA	1008	A	C5-N7-C8	6.83	107.32	103.90
22	BA	1746	A	C4-C5-C6	6.83	120.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	687	A	C4-C5-C6	6.83	120.42	117.00
22	BA	983	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1634	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1586	A	C5-N7-C8	6.83	107.31	103.90
1	AA	8	A	C8-N9-C4	6.83	108.53	105.80
1	AA	539	A	N3-C4-N9	6.83	132.86	127.40
22	BA	1504	A	C8-N9-C4	6.83	108.53	105.80
22	BA	508	A	N3-C4-N9	6.82	132.86	127.40
1	AA	69	G	O5'-C5'-C4'	-6.82	98.74	111.70
1	AA	430	A	C8-N9-C4	6.82	108.53	105.80
22	BA	693	A	N3-C4-N9	6.82	132.86	127.40
22	BA	2899	A	C8-N9-C4	6.82	108.53	105.80
22	BA	632	A	N3-C4-N9	6.82	132.85	127.40
22	BA	2449	U	C5-C4-O4	-6.82	121.81	125.90
1	AA	814	A	C5-N7-C8	6.82	107.31	103.90
1	AA	923	A	N3-C4-N9	6.82	132.85	127.40
1	AA	1004	A	C4-C5-C6	6.82	120.41	117.00
22	BA	309	A	C4-C5-C6	6.82	120.41	117.00
22	BA	750	A	C8-N9-C4	6.82	108.53	105.80
22	BA	1515	A	N9-C4-C5	6.82	108.53	105.80
22	BA	1953	A	C5-N7-C8	6.82	107.31	103.90
22	BA	2639	A	C5-C6-N1	6.82	121.11	117.70
1	AA	1418	A	C5-N7-C8	6.82	107.31	103.90
1	AA	1179	A	C4-C5-N7	-6.81	107.29	110.70
1	AA	1531	A	C4-C5-C6	6.81	120.41	117.00
22	BA	453	A	C4-C5-C6	6.81	120.41	117.00
22	BA	1755	A	C8-N9-C4	6.81	108.53	105.80
22	BA	2734	A	N9-C4-C5	6.81	108.53	105.80
1	AA	502	A	C5-N7-C8	6.81	107.31	103.90
22	BA	480	A	N3-C4-N9	6.81	132.85	127.40
22	BA	789	A	C5-C6-N1	6.81	121.11	117.70
22	BA	1384	A	C4-C5-C6	6.81	120.40	117.00
1	AA	456	A	C4-C5-C6	6.81	120.40	117.00
22	BA	1431	A	N3-C4-N9	6.81	132.84	127.40
1	AA	253	A	C8-N9-C4	6.80	108.52	105.80
1	AA	1324	A	C4-C5-C6	6.80	120.40	117.00
22	BA	131	A	C5-N7-C8	6.80	107.30	103.90
22	BA	161	A	C8-N9-C4	6.80	108.52	105.80
22	BA	1000	A	C5-N7-C8	6.80	107.30	103.90
22	BA	1147	A	N9-C4-C5	6.80	108.52	105.80
1	AA	465	A	N3-C4-N9	6.80	132.84	127.40
1	AA	1513	A	N3-C4-N9	6.80	132.84	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	131	A	C4-C5-C6	6.80	120.40	117.00
1	AA	687	A	C8-N9-C4	6.80	108.52	105.80
1	AA	1005	A	C4-C5-C6	6.80	120.40	117.00
22	BA	764	A	C8-N9-C4	6.80	108.52	105.80
1	AA	298	A	C8-N9-C4	6.80	108.52	105.80
1	AA	1201	A	C5-C6-N1	6.80	121.10	117.70
22	BA	119	A	N9-C4-C5	6.80	108.52	105.80
22	BA	1626	A	C5-N7-C8	6.80	107.30	103.90
22	BA	2163	A	C8-N9-C4	6.80	108.52	105.80
22	BA	324	A	C5-N7-C8	6.79	107.30	103.90
22	BA	2288	A	C8-N9-C4	6.79	108.52	105.80
22	BA	447	A	N3-C4-N9	6.79	132.84	127.40
1	AA	101	A	N3-C4-N9	6.79	132.83	127.40
1	AA	174	A	N9-C4-C5	6.79	108.52	105.80
1	AA	629	A	C4-C5-C6	6.79	120.39	117.00
22	BA	1613	G	C6-C5-N7	6.79	134.47	130.40
22	BA	1745	A	C4-C5-C6	6.79	120.39	117.00
22	BA	2317	A	N3-C4-N9	6.79	132.83	127.40
22	BA	2142	A	N3-C4-N9	6.79	132.83	127.40
1	AA	1428	A	N9-C4-C5	6.79	108.51	105.80
22	BA	146	A	N3-C4-N9	6.79	132.83	127.40
22	BA	739	A	N3-C4-N9	6.79	132.83	127.40
22	BA	2278	A	C4-C5-C6	6.79	120.39	117.00
1	AA	642	A	C4-C5-C6	6.78	120.39	117.00
1	AA	1513	A	C8-N9-C4	6.78	108.51	105.80
22	BA	1262	A	N9-C4-C5	6.78	108.51	105.80
22	BA	1307	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1191	A	C5-N7-C8	6.78	107.29	103.90
22	BA	1469	A	C8-N9-C4	6.78	108.51	105.80
22	BA	959	A	C4-C5-C6	6.78	120.39	117.00
22	BA	2070	A	N9-C4-C5	6.78	108.51	105.80
22	BA	2734	A	C4-C5-C6	6.78	120.39	117.00
22	BA	1275	A	N3-C4-N9	6.77	132.82	127.40
22	BA	2183	A	C4-C5-C6	6.77	120.39	117.00
22	BA	621	A	C5-N7-C8	6.77	107.29	103.90
1	AA	946	A	N3-C4-N9	6.77	132.82	127.40
22	BA	44	A	C4-C5-C6	6.77	120.39	117.00
1	AA	1055	A	C4-C5-C6	6.77	120.38	117.00
22	BA	643	A	N3-C4-N9	6.77	132.81	127.40
22	BA	1739	A	N3-C4-N9	6.77	132.81	127.40
22	BA	2386	A	N3-C4-N9	6.77	132.81	127.40
1	AA	1197	A	C5-N7-C8	6.76	107.28	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	111	A	N9-C4-C5	6.76	108.51	105.80
22	BA	146	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2042	A	C5-N7-C8	6.76	107.28	103.90
22	BA	2042	A	N3-C4-N9	6.76	132.81	127.40
1	AA	313	A	N3-C4-N9	6.76	132.81	127.40
22	BA	2080	A	C8-N9-C4	6.76	108.50	105.80
22	BA	2135	A	N9-C4-C5	6.76	108.50	105.80
1	AA	496	A	C5-N7-C8	6.76	107.28	103.90
1	AA	1332	A	C5-N7-C8	6.76	107.28	103.90
22	BA	311	A	C4-C5-C6	6.76	120.38	117.00
22	BA	1254	A	C8-N9-C4	6.76	108.50	105.80
1	AA	964	A	N3-C4-N9	6.76	132.81	127.40
22	BA	5	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2430	A	N9-C4-C5	6.76	108.50	105.80
1	AA	499	A	C8-N9-C4	6.75	108.50	105.80
22	BA	1367	A	C8-N9-C4	6.75	108.50	105.80
22	BA	2566	A	C5-N7-C8	6.75	107.28	103.90
1	AA	441	A	N3-C4-N9	6.75	132.80	127.40
1	AA	792	A	C5-C6-N1	6.75	121.08	117.70
1	AA	873	A	N3-C4-N9	6.75	132.80	127.40
22	BA	21	A	N3-C4-N9	6.75	132.80	127.40
22	BA	84	A	C5-N7-C8	6.75	107.28	103.90
22	BA	655	A	C8-N9-C4	6.75	108.50	105.80
22	BA	2453	A	C5-N7-C8	6.75	107.28	103.90
1	AA	288	A	C5-N7-C8	6.75	107.27	103.90
1	AA	466	A	C4-C5-C6	6.75	120.37	117.00
22	BA	181	A	N9-C4-C5	6.75	108.50	105.80
22	BA	781	A	N3-C4-N9	6.75	132.80	127.40
1	AA	167	A	C8-N9-C4	6.75	108.50	105.80
1	AA	1169	A	C4-C5-C6	6.75	120.37	117.00
22	BA	2014	A	C5-N7-C8	6.75	107.27	103.90
1	AA	250	A	C8-N9-C4	6.74	108.50	105.80
22	BA	2868	A	N3-C4-N9	6.74	132.79	127.40
22	BA	345	A	C4-C5-C6	6.74	120.37	117.00
22	BA	2675	A	C5-C6-N1	6.74	121.07	117.70
1	AA	767	A	C5-N7-C8	6.74	107.27	103.90
22	BA	2176	A	N3-C4-N9	6.74	132.79	127.40
1	AA	609	A	N3-C4-N9	6.74	132.79	127.40
1	AA	712	A	N3-C4-N9	6.74	132.79	127.40
1	AA	1468	A	C8-N9-C4	6.74	108.50	105.80
22	BA	1960	A	C5-N7-C8	6.74	107.27	103.90
1	AA	1413	A	C8-N9-C4	6.74	108.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	905	A	C4-C5-C6	6.74	120.37	117.00
22	BA	1613	G	C5-C6-O6	6.74	132.64	128.60
1	AA	673	A	C4-C5-C6	6.74	120.37	117.00
22	BA	1069	A	C4-C5-C6	6.74	120.37	117.00
22	BA	504	A	N3-C4-N9	6.73	132.79	127.40
22	BA	1503	A	N9-C4-C5	6.73	108.49	105.80
1	AA	32	A	C5-C6-N1	6.73	121.07	117.70
1	AA	238	A	C4-C5-C6	6.73	120.37	117.00
1	AA	794	A	C4-C5-C6	6.73	120.37	117.00
22	BA	2117	A	N3-C4-N9	6.73	132.78	127.40
22	BA	2598	A	C5-N7-C8	6.73	107.27	103.90
1	AA	160	A	C5-C6-N1	6.73	121.06	117.70
1	AA	977	A	N3-C4-N9	6.73	132.78	127.40
22	BA	167	A	N3-C4-N9	6.73	132.78	127.40
22	BA	172	A	C4-C5-C6	6.73	120.36	117.00
22	BA	173	A	C5-N7-C8	6.73	107.27	103.90
22	BA	354	A	C8-N9-C4	6.73	108.49	105.80
22	BA	1050	A	C4-C5-C6	6.73	120.36	117.00
1	AA	243	A	C4-C5-N7	-6.73	107.33	110.70
1	AA	825	A	C5-C6-N1	6.73	121.06	117.70
22	BA	730	A	N3-C4-N9	6.73	132.78	127.40
22	BA	1495	A	C5-N7-C8	6.73	107.26	103.90
1	AA	1191	A	C4-C5-C6	6.72	120.36	117.00
22	BA	1579	A	C8-N9-C4	6.72	108.49	105.80
22	BA	1789	A	N3-C4-N9	6.72	132.78	127.40
22	BA	1901	A	C5-N7-C8	6.72	107.26	103.90
1	AA	309	A	C8-N9-C4	6.72	108.49	105.80
1	AA	161	A	N3-C4-N9	6.72	132.78	127.40
22	BA	1260	A	C5-N7-C8	6.72	107.26	103.90
22	BA	2430	A	N3-C4-C5	-6.72	122.10	126.80
55	B8	26	A	C4-C5-C6	6.72	120.36	117.00
1	AA	906	A	C8-N9-C4	6.72	108.49	105.80
22	BA	2478	A	C5-N7-C8	6.72	107.26	103.90
1	AA	784	A	N3-C4-N9	6.72	132.77	127.40
22	BA	1147	A	C5-C6-N1	6.72	121.06	117.70
22	BA	2541	A	C8-N9-C4	6.72	108.49	105.80
1	AA	329	A	C8-N9-C4	6.71	108.49	105.80
22	BA	802	A	N9-C4-C5	6.71	108.49	105.80
22	BA	920	A	N3-C4-N9	6.71	132.77	127.40
22	BA	2170	A	C8-N9-C4	6.71	108.49	105.80
22	BA	255	A	C5-N7-C8	6.71	107.26	103.90
22	BA	693	A	C8-N9-C4	6.71	108.48	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	933	A	C4-C5-C6	6.71	120.36	117.00
22	BA	1048	A	C4-C5-C6	6.71	120.36	117.00
22	BA	1434	A	N3-C4-N9	6.71	132.77	127.40
22	BA	1142	A	N3-C4-N9	6.71	132.77	127.40
1	AA	44	A	N9-C4-C5	6.71	108.48	105.80
22	BA	443	A	C5-N7-C8	6.71	107.25	103.90
22	BA	574	A	N3-C4-N9	6.71	132.77	127.40
22	BA	1847	A	N3-C4-N9	6.71	132.77	127.40
22	BA	945	A	C4-C5-C6	6.71	120.35	117.00
1	AA	192	A	N9-C4-C5	6.70	108.48	105.80
22	BA	2461	A	C8-N9-C4	6.70	108.48	105.80
1	AA	487	A	C8-N9-C4	6.70	108.48	105.80
22	BA	2721	A	N3-C4-N9	6.70	132.76	127.40
22	BA	2376	A	C8-N9-C4	6.70	108.48	105.80
22	BA	497	A	C8-N9-C4	6.70	108.48	105.80
22	BA	1151	A	N3-C4-N9	6.69	132.75	127.40
22	BA	2284	A	C5-N7-C8	6.69	107.25	103.90
22	BA	2738	A	C5-N7-C8	6.69	107.25	103.90
1	AA	408	A	C4-C5-C6	6.69	120.35	117.00
22	BA	5	A	C8-N9-C4	6.69	108.48	105.80
22	BA	1978	A	C5-C6-N1	6.69	121.05	117.70
1	AA	747	A	C4-C5-C6	6.69	120.34	117.00
22	BA	735	A	C4-C5-C6	6.69	120.34	117.00
22	BA	1987	A	C4-C5-C6	6.69	120.34	117.00
22	BA	675	A	C8-N9-C4	6.69	108.48	105.80
22	BA	704	G	O4'-C1'-N9	6.69	113.55	108.20
1	AA	371	A	C8-N9-C4	6.69	108.47	105.80
1	AA	1081	A	N3-C4-N9	6.69	132.75	127.40
22	BA	401	A	C5-N7-C8	6.69	107.24	103.90
22	BA	1932	A	C4-C5-C6	6.69	120.34	117.00
1	AA	768	A	N3-C4-N9	6.69	132.75	127.40
1	AA	583	A	N9-C4-C5	6.68	108.47	105.80
1	AA	1170	A	C8-N9-C4	6.68	108.47	105.80
22	BA	996	A	C8-N9-C4	6.68	108.47	105.80
22	BA	1226	A	N3-C4-N9	6.68	132.75	127.40
1	AA	1170	A	N3-C4-N9	6.68	132.75	127.40
1	AA	753	A	C8-N9-C4	6.68	108.47	105.80
22	BA	1969	A	C8-N9-C4	6.68	108.47	105.80
1	AA	228	A	C4-C5-C6	6.68	120.34	117.00
1	AA	288	A	C8-N9-C4	6.68	108.47	105.80
1	AA	729	A	N9-C4-C5	6.68	108.47	105.80
22	BA	2461	A	C5-C6-N1	6.68	121.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	814	A	C8-N9-C4	6.68	108.47	105.80
22	BA	1470	A	N3-C4-N9	6.68	132.74	127.40
22	BA	2448	A	N9-C4-C5	6.68	108.47	105.80
22	BA	131	A	C4-C5-C6	6.67	120.34	117.00
22	BA	480	A	C4-C5-C6	6.67	120.34	117.00
22	BA	727	A	C8-N9-C4	6.67	108.47	105.80
22	BA	1246	A	N3-C4-N9	6.67	132.74	127.40
22	BA	2531	A	N3-C4-N9	6.67	132.74	127.40
1	AA	702	A	C5-N7-C8	6.67	107.24	103.90
1	AA	1287	A	C4-C5-C6	6.67	120.34	117.00
22	BA	693	A	C4-C5-C6	6.67	120.34	117.00
22	BA	1147	A	C4-C5-N7	-6.67	107.36	110.70
22	BA	2126	A	C8-N9-C4	6.67	108.47	105.80
22	BA	278	A	N3-C4-N9	6.67	132.74	127.40
22	BA	439	A	N3-C4-N9	6.67	132.73	127.40
22	BA	1431	A	C8-N9-C4	6.67	108.47	105.80
22	BA	1754	A	C5-N7-C8	6.67	107.23	103.90
22	BA	909	A	C5-N7-C8	6.67	107.23	103.90
1	AA	554	A	C4-C5-N7	-6.67	107.37	110.70
1	AA	1035	A	N3-C4-N9	6.67	132.73	127.40
1	AA	1275	A	C4-C5-C6	6.67	120.33	117.00
22	BA	1801	A	N3-C4-N9	6.66	132.73	127.40
22	BA	2328	A	N3-C4-N9	6.66	132.73	127.40
22	BA	1028	A	C5-N7-C8	6.66	107.23	103.90
22	BA	1189	A	C8-N9-C4	6.66	108.46	105.80
22	BA	2887	A	C5-N7-C8	6.66	107.23	103.90
23	BB	45	A	N3-C4-N9	6.66	132.73	127.40
1	AA	306	A	C8-N9-C4	6.66	108.46	105.80
22	BA	781	A	C8-N9-C4	6.66	108.46	105.80
22	BA	911	A	N3-C4-N9	6.66	132.73	127.40
22	BA	1308	A	C4-C5-N7	-6.66	107.37	110.70
22	BA	1552	A	N3-C4-N9	6.66	132.73	127.40
22	BA	1928	A	C4-C5-C6	6.66	120.33	117.00
22	BA	2738	A	C4-C5-C6	6.66	120.33	117.00
1	AA	696	A	N3-C4-N9	6.66	132.72	127.40
1	AA	1035	A	N9-C4-C5	6.66	108.46	105.80
1	AA	715	A	N3-C4-N9	6.66	132.72	127.40
22	BA	430	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1383	A	N3-C4-N9	6.66	132.72	127.40
22	BA	1433	A	C5-N7-C8	6.66	107.23	103.90
22	BA	1871	A	C8-N9-C4	6.66	108.46	105.80
22	BA	2051	A	C5-N7-C8	6.66	107.23	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2059	A	C5-C6-N1	6.66	121.03	117.70
22	BA	2412	A	C4-C5-C6	6.66	120.33	117.00
22	BA	227	A	C8-N9-C4	6.65	108.46	105.80
22	BA	750	A	C4-C5-C6	6.65	120.33	117.00
1	AA	718	A	C4-C5-C6	6.65	120.33	117.00
22	BA	2432	A	N3-C4-N9	6.65	132.72	127.40
1	AA	908	A	C4-C5-C6	6.65	120.33	117.00
22	BA	149	A	C4-C5-C6	6.65	120.33	117.00
22	BA	1508	A	N3-C4-N9	6.65	132.72	127.40
1	AA	53	A	N3-C4-N9	6.65	132.72	127.40
1	AA	151	A	C4-C5-C6	6.65	120.32	117.00
22	BA	111	A	C4-C5-N7	-6.65	107.38	110.70
22	BA	1098	A	C8-N9-C4	6.65	108.46	105.80
22	BA	975	A	C4-C5-C6	6.65	120.32	117.00
1	AA	452	A	C4-C5-C6	6.64	120.32	117.00
1	AA	640	A	C5-N7-C8	6.64	107.22	103.90
1	AA	746	A	C5-C6-N1	6.64	121.02	117.70
1	AA	1363	A	N3-C4-N9	6.64	132.72	127.40
22	BA	933	A	N3-C4-N9	6.64	132.72	127.40
22	BA	2058	A	N9-C4-C5	6.64	108.46	105.80
1	AA	72	A	C8-N9-C4	6.64	108.46	105.80
1	AA	780	A	N3-C4-N9	6.64	132.71	127.40
1	AA	946	A	C4-C5-C6	6.64	120.32	117.00
1	AA	1102	A	C8-N9-C4	6.64	108.46	105.80
22	BA	1088	A	N3-C4-N9	6.64	132.71	127.40
1	AA	1513	A	C4-C5-C6	6.64	120.32	117.00
22	BA	526	A	C4-C5-N7	-6.64	107.38	110.70
22	BA	722	A	C8-N9-C4	6.64	108.46	105.80
22	BA	1952	A	C8-N9-C4	6.64	108.46	105.80
1	AA	262	A	N3-C4-N9	6.64	132.71	127.40
22	BA	1654	A	C4-C5-C6	6.64	120.32	117.00
22	BA	2433	A	C5-N7-C8	6.64	107.22	103.90
1	AA	71	A	C8-N9-C4	6.64	108.45	105.80
22	BA	49	A	C4-C5-C6	6.64	120.32	117.00
22	BA	345	A	N3-C4-N9	6.64	132.71	127.40
22	BA	733	G	C4-C5-N7	6.64	113.45	110.80
22	BA	173	A	N3-C4-N9	6.63	132.71	127.40
22	BA	428	A	N3-C4-N9	6.63	132.71	127.40
22	BA	466	A	C8-N9-C4	6.63	108.45	105.80
22	BA	1384	A	C8-N9-C4	6.63	108.45	105.80
1	AA	205	A	N3-C4-N9	6.63	132.71	127.40
1	AA	1499	A	N3-C4-N9	6.63	132.71	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1532	A	C8-N9-C4	6.63	108.45	105.80
22	BA	2015	A	N3-C4-N9	6.63	132.71	127.40
22	BA	14	A	N9-C4-C5	6.63	108.45	105.80
22	BA	627	A	N3-C4-N9	6.63	132.70	127.40
22	BA	1885	A	N3-C4-N9	6.63	132.70	127.40
1	AA	663	A	C4-C5-C6	6.63	120.31	117.00
1	AA	1375	A	N3-C4-N9	6.63	132.70	127.40
55	B8	59	A	C4-C5-C6	6.63	120.31	117.00
1	AA	1324	A	C8-N9-C4	6.63	108.45	105.80
3	AC	107	ARG	CG-CD-NE	6.63	125.72	111.80
22	BA	1073	A	N3-C4-N9	6.63	132.70	127.40
1	AA	1318	A	C5-N7-C8	6.62	107.21	103.90
22	BA	2469	A	C5-N7-C8	6.62	107.21	103.90
22	BA	104	A	C4-C5-C6	6.62	120.31	117.00
22	BA	508	A	C4-C5-C6	6.62	120.31	117.00
22	BA	547	A	N3-C4-N9	6.62	132.70	127.40
22	BA	1020	A	C5-N7-C8	6.62	107.21	103.90
22	BA	1048	A	C8-N9-C4	6.62	108.45	105.80
22	BA	1384	A	N3-C4-N9	6.62	132.70	127.40
22	BA	126	A	N9-C4-C5	6.62	108.45	105.80
22	BA	2054	A	N9-C4-C5	6.62	108.45	105.80
1	AA	1081	A	C4-C5-C6	6.62	120.31	117.00
1	AA	1441	A	C8-N9-C4	6.62	108.45	105.80
1	AA	363	A	C8-N9-C4	6.61	108.44	105.80
1	AA	1152	A	C5-N7-C8	6.61	107.21	103.90
22	BA	146	A	C5-C6-N1	6.61	121.01	117.70
22	BA	1040	A	N3-C4-N9	6.61	132.69	127.40
1	AA	149	A	N9-C4-C5	6.61	108.44	105.80
22	BA	104	A	N3-C4-N9	6.61	132.69	127.40
22	BA	2158	A	N3-C4-N9	6.61	132.69	127.40
22	BA	2411	A	C8-N9-C4	6.61	108.44	105.80
1	AA	1252	A	N3-C4-N9	6.61	132.69	127.40
22	BA	1745	A	C8-N9-C4	6.61	108.44	105.80
22	BA	2837	A	N9-C4-C5	6.61	108.44	105.80
1	AA	349	A	N9-C4-C5	6.61	108.44	105.80
22	BA	152	A	C8-N9-C4	6.61	108.44	105.80
22	BA	1089	A	C8-N9-C4	6.61	108.44	105.80
1	AA	1150	A	C8-N9-C4	6.61	108.44	105.80
23	BB	45	A	C4-C5-N7	-6.61	107.40	110.70
22	BA	988	A	C8-N9-C4	6.60	108.44	105.80
1	AA	468	A	C4-C5-C6	6.60	120.30	117.00
1	AA	1229	A	N9-C4-C5	6.60	108.44	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1428	A	C4-C5-N7	-6.60	107.40	110.70
22	BA	127	A	C8-N9-C4	6.60	108.44	105.80
22	BA	920	A	C8-N9-C4	6.60	108.44	105.80
22	BA	2733	A	C4-C5-C6	6.60	120.30	117.00
22	BA	2778	A	N3-C4-N9	6.60	132.68	127.40
22	BA	945	A	C5-C6-N1	6.60	121.00	117.70
22	BA	262	A	C8-N9-C4	6.60	108.44	105.80
1	AA	1	A	C4-C5-C6	6.59	120.30	117.00
1	AA	160	A	C4-C5-N7	-6.59	107.40	110.70
1	AA	794	A	N3-C4-N9	6.59	132.68	127.40
22	BA	324	A	C5-C6-N1	6.59	121.00	117.70
22	BA	1522	A	C8-N9-C4	6.59	108.44	105.80
22	BA	1616	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1805	A	C4-C5-N7	-6.59	107.40	110.70
22	BA	727	A	N3-C4-N9	6.59	132.67	127.40
1	AA	306	A	N3-C4-N9	6.59	132.67	127.40
22	BA	1496	A	C5-N7-C8	6.59	107.19	103.90
22	BA	1571	A	N3-C4-N9	6.59	132.67	127.40
22	BA	2227	A	N9-C4-C5	6.59	108.44	105.80
55	B8	69	A	C4-C5-C6	6.59	120.30	117.00
1	AA	860	A	C8-N9-C4	6.59	108.44	105.80
1	AA	1406	U	C2-N3-C4	-6.59	123.05	127.00
22	BA	482	A	N3-C4-N9	6.59	132.67	127.40
22	BA	1253	A	N9-C4-C5	6.58	108.43	105.80
23	BB	108	A	C4-C5-C6	6.58	120.29	117.00
1	AA	716	A	N3-C4-N9	6.58	132.67	127.40
1	AA	1333	A	C4-C5-N7	-6.58	107.41	110.70
22	BA	892	A	N3-C4-N9	6.58	132.67	127.40
22	BA	1610	A	N3-C4-N9	6.58	132.67	127.40
22	BA	2872	A	C6-N1-C2	6.58	122.55	118.60
1	AA	3	A	C4-C5-C6	6.58	120.29	117.00
22	BA	1269	A	C5-C6-N1	6.58	120.99	117.70
22	BA	1321	A	N9-C4-C5	6.58	108.43	105.80
22	BA	2809	A	C5-N7-C8	6.58	107.19	103.90
22	BA	2820	A	C8-N9-C4	6.58	108.43	105.80
1	AA	95	C	C2-N1-C1'	6.58	126.04	118.80
1	AA	1238	A	N3-C4-N9	6.58	132.66	127.40
22	BA	460	A	C4-C5-C6	6.58	120.29	117.00
1	AA	19	A	C5-C6-N1	6.58	120.99	117.70
1	AA	238	A	N9-C4-C5	6.58	108.43	105.80
1	AA	563	A	N3-C4-N9	6.58	132.66	127.40
1	AA	865	A	N3-C4-N9	6.58	132.66	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	654	A	C8-N9-C4	6.58	108.43	105.80
1	AA	1447	A	C8-N9-C4	6.58	108.43	105.80
22	BA	2183	A	N3-C4-N9	6.58	132.66	127.40
22	BA	182	A	C4-C5-C6	6.57	120.29	117.00
22	BA	863	A	N3-C4-N9	6.57	132.66	127.40
22	BA	996	A	C4-C5-C6	6.57	120.29	117.00
22	BA	1020	A	C4-C5-C6	6.57	120.29	117.00
22	BA	2060	A	C8-N9-C4	6.57	108.43	105.80
54	B7	9	A	N3-C4-N9	6.57	132.66	127.40
22	BA	2005	A	N3-C4-N9	6.57	132.66	127.40
1	AA	32	A	C4-C5-C6	6.57	120.28	117.00
1	AA	878	A	N3-C4-N9	6.57	132.66	127.40
1	AA	975	A	N3-C4-N9	6.57	132.66	127.40
1	AA	1269	A	C8-N9-C4	6.57	108.43	105.80
22	BA	2014	A	C4-C5-C6	6.57	120.28	117.00
22	BA	2309	A	C8-N9-C4	6.57	108.43	105.80
22	BA	2471	A	C8-N9-C4	6.57	108.43	105.80
22	BA	160	A	C8-N9-C4	6.57	108.43	105.80
22	BA	5	A	N3-C4-N9	6.57	132.65	127.40
22	BA	156	A	N3-C4-N9	6.57	132.65	127.40
22	BA	219	A	N3-C4-N9	6.57	132.65	127.40
22	BA	990	A	C8-N9-C4	6.57	108.43	105.80
22	BA	1780	A	N3-C4-N9	6.57	132.65	127.40
22	BA	256	A	N3-C4-N9	6.57	132.65	127.40
22	BA	1551	A	N9-C4-C5	6.57	108.43	105.80
23	BB	73	A	N3-C4-N9	6.57	132.65	127.40
1	AA	1332	A	C8-N9-C4	6.56	108.43	105.80
1	AA	1311	A	C4-C5-C6	6.56	120.28	117.00
22	BA	1597	A	N3-C4-N9	6.56	132.65	127.40
22	BA	2813	A	N3-C4-N9	6.56	132.65	127.40
22	BA	382	A	N3-C4-N9	6.56	132.65	127.40
22	BA	675	A	N3-C4-N9	6.56	132.65	127.40
22	BA	1067	A	C8-N9-C4	6.56	108.42	105.80
22	BA	2019	A	C8-N9-C4	6.56	108.42	105.80
22	BA	2900	A	N9-C4-C5	6.56	108.42	105.80
55	B8	73	A	N9-C4-C5	6.56	108.42	105.80
1	AA	270	A	N3-C4-N9	6.56	132.65	127.40
1	AA	1005	A	N3-C4-N9	6.56	132.65	127.40
1	AA	1500	A	N3-C4-N9	6.56	132.65	127.40
22	BA	2497	A	N3-C4-N9	6.56	132.65	127.40
22	BA	275	C	C2-N1-C1'	-6.56	111.59	118.80
22	BA	2391	G	O4'-C1'-N9	6.56	113.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1306	A	C4-C5-C6	6.55	120.28	117.00
22	BA	1086	A	C4-C5-C6	6.55	120.28	117.00
22	BA	1129	A	C8-N9-C4	6.55	108.42	105.80
22	BA	1889	A	N3-C4-N9	6.55	132.64	127.40
55	B8	76	A	C4-C5-C6	6.55	120.28	117.00
1	AA	74	A	C4-C5-N7	-6.55	107.42	110.70
1	AA	155	A	C8-N9-C4	6.55	108.42	105.80
22	BA	1525	A	N9-C4-C5	6.55	108.42	105.80
22	BA	1876	A	C4-C5-C6	6.55	120.28	117.00
1	AA	547	A	N9-C4-C5	6.55	108.42	105.80
1	AA	1157	A	C4-C5-C6	6.55	120.28	117.00
1	AA	1339	A	N3-C4-N9	6.55	132.64	127.40
22	BA	673	C	N3-C4-C5	6.55	124.52	121.90
22	BA	896	A	C4-C5-C6	6.55	120.27	117.00
22	BA	2071	A	N3-C4-N9	6.55	132.64	127.40
1	AA	918	A	N9-C4-C5	6.55	108.42	105.80
1	AA	878	A	C4-C5-C6	6.55	120.27	117.00
22	BA	541	A	C8-N9-C4	6.55	108.42	105.80
22	BA	1284	A	C4-C5-C6	6.55	120.27	117.00
1	AA	718	A	N3-C4-N9	6.54	132.64	127.40
1	AA	608	A	N3-C4-N9	6.54	132.63	127.40
22	BA	384	A	C4-C5-C6	6.54	120.27	117.00
1	AA	539	A	C8-N9-C4	6.54	108.42	105.80
22	BA	1548	A	C5-C6-N1	6.54	120.97	117.70
22	BA	2212	A	N3-C4-N9	6.54	132.63	127.40
1	AA	131	A	N3-C4-N9	6.54	132.63	127.40
22	BA	547	A	C4-C5-C6	6.54	120.27	117.00
1	AA	1507	A	C5-C6-N1	6.54	120.97	117.70
22	BA	877	A	N3-C4-N9	6.54	132.63	127.40
1	AA	913	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1502	A	C8-N9-C4	6.54	108.41	105.80
22	BA	1665	A	N9-C4-C5	6.54	108.41	105.80
22	BA	1744	A	C4-C5-C6	6.53	120.27	117.00
22	BA	2654	A	C4-C5-C6	6.53	120.27	117.00
22	BA	2333	A	C8-N9-C4	6.53	108.41	105.80
1	AA	743	A	C4-C5-C6	6.53	120.27	117.00
1	AA	872	A	N3-C4-N9	6.53	132.62	127.40
1	AA	1213	A	C4-C5-N7	-6.53	107.44	110.70
22	BA	21	A	C4-C5-C6	6.53	120.27	117.00
22	BA	1373	A	C5-C6-N1	6.53	120.97	117.70
22	BA	2288	A	C4-C5-C6	6.53	120.27	117.00
1	AA	825	A	C8-N9-C4	6.53	108.41	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	428	A	C4-C5-C6	6.53	120.26	117.00
22	BA	1353	A	N9-C4-C5	6.53	108.41	105.80
22	BA	2893	A	C8-N9-C4	6.53	108.41	105.80
1	AA	1201	A	C5-C6-N6	6.53	128.92	123.70
22	BA	1077	A	C4-C5-C6	6.53	120.26	117.00
22	BA	1156	A	C4-C5-C6	6.53	120.26	117.00
22	BA	2469	A	C5-C6-N1	6.53	120.96	117.70
22	BA	2705	A	C4-C5-C6	6.53	120.26	117.00
1	AA	68	G	C8-N9-C1'	-6.52	118.52	127.00
22	BA	1535	A	N9-C4-C5	6.52	108.41	105.80
22	BA	2205	A	N3-C4-N9	6.52	132.62	127.40
22	BA	2247	A	N3-C4-N9	6.52	132.62	127.40
1	AA	1324	A	N3-C4-N9	6.52	132.62	127.40
1	AA	583	A	C8-N9-C4	6.52	108.41	105.80
22	BA	1387	A	C5-C6-N1	6.52	120.96	117.70
22	BA	1783	A	C4-C5-N7	-6.52	107.44	110.70
22	BA	144	A	N9-C4-C5	6.52	108.41	105.80
1	AA	1004	A	C8-N9-C4	6.51	108.41	105.80
1	AA	1036	A	C8-N9-C4	6.51	108.41	105.80
22	BA	522	A	C5-C6-N1	6.51	120.96	117.70
22	BA	1502	A	N3-C4-N9	6.51	132.61	127.40
22	BA	2547	A	C4-C5-C6	6.51	120.26	117.00
1	AA	236	A	C4-C5-C6	6.51	120.26	117.00
1	AA	532	A	C8-N9-C4	6.51	108.40	105.80
22	BA	2281	A	C8-N9-C4	6.51	108.41	105.80
1	AA	622	A	N9-C4-C5	6.51	108.40	105.80
1	AA	1492	A	N9-C4-C5	6.51	108.40	105.80
22	BA	2682	A	N3-C4-N9	6.51	132.61	127.40
22	BA	1549	A	C8-N9-C4	6.51	108.40	105.80
1	AA	509	A	C4-C5-C6	6.51	120.25	117.00
1	AA	964	A	C8-N9-C4	6.51	108.40	105.80
22	BA	1597	A	C5-C6-N1	6.51	120.95	117.70
22	BA	2184	A	N3-C4-N9	6.51	132.60	127.40
22	BA	472	A	C5-N7-C8	6.50	107.15	103.90
22	BA	1735	A	C4-C5-C6	6.50	120.25	117.00
22	BA	2051	A	C4-C5-C6	6.50	120.25	117.00
1	AA	325	A	C4-C5-C6	6.50	120.25	117.00
22	BA	368	A	C8-N9-C4	6.50	108.40	105.80
22	BA	1717	A	C8-N9-C4	6.50	108.40	105.80
1	AA	1251	A	N9-C4-C5	6.50	108.40	105.80
22	BA	412	A	N3-C4-N9	6.50	132.60	127.40
22	BA	1129	A	N3-C4-N9	6.50	132.60	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1794	A	C5-C6-N1	6.50	120.95	117.70
22	BA	1998	A	C4-C5-N7	-6.50	107.45	110.70
22	BA	2448	A	C4-C5-N7	-6.50	107.45	110.70
22	BA	503	A	C5-N7-C8	6.50	107.15	103.90
22	BA	1214	A	C5-N7-C8	6.50	107.15	103.90
22	BA	56	A	C8-N9-C4	6.50	108.40	105.80
22	BA	196	A	C8-N9-C4	6.50	108.40	105.80
22	BA	608	A	N3-C4-N9	6.50	132.60	127.40
22	BA	1347	A	C4-C5-C6	6.49	120.25	117.00
22	BA	1608	A	C4-C5-C6	6.49	120.25	117.00
22	BA	2435	A	C4-C5-N7	-6.49	107.45	110.70
22	BA	21	A	C8-N9-C4	6.49	108.40	105.80
22	BA	439	A	C4-C5-C6	6.49	120.25	117.00
22	BA	2447	G	C5-C6-N1	6.49	114.75	111.50
1	AA	1492	A	C4-C5-C6	6.49	120.25	117.00
1	AA	466	A	N9-C4-C5	6.49	108.39	105.80
1	AA	1176	A	C4-C5-C6	6.49	120.24	117.00
22	BA	825	A	C4-C5-N7	-6.49	107.46	110.70
1	AA	262	A	C4-C5-C6	6.49	120.24	117.00
1	AA	676	A	C8-N9-C4	6.49	108.39	105.80
22	BA	119	A	C5-N7-C8	6.49	107.14	103.90
22	BA	404	A	C8-N9-C4	6.49	108.39	105.80
22	BA	670	A	N3-C4-N9	6.49	132.59	127.40
22	BA	742	A	C4-C5-C6	6.49	120.24	117.00
22	BA	918	A	C5-N7-C8	6.49	107.14	103.90
22	BA	2418	A	C8-N9-C4	6.49	108.39	105.80
1	AA	1019	A	C4-C5-C6	6.48	120.24	117.00
22	BA	1433	A	C8-N9-C4	6.48	108.39	105.80
22	BA	2080	A	N3-C4-N9	6.48	132.59	127.40
1	AA	270	A	C5-C6-N1	6.48	120.94	117.70
22	BA	1086	A	C4-C5-N7	-6.48	107.46	110.70
22	BA	1439	A	N3-C4-N9	6.48	132.59	127.40
22	BA	2080	A	C5-C6-N1	6.48	120.94	117.70
22	BA	2740	A	C4-C5-C6	6.48	120.24	117.00
1	AA	702	A	N3-C4-N9	6.48	132.58	127.40
22	BA	430	A	C8-N9-C4	6.48	108.39	105.80
22	BA	1021	A	N9-C4-C5	6.48	108.39	105.80
22	BA	182	A	N3-C4-N9	6.48	132.58	127.40
22	BA	2191	A	N3-C4-N9	6.48	132.58	127.40
1	AA	246	A	C4-C5-C6	6.48	120.24	117.00
1	AA	559	A	N3-C4-N9	6.48	132.58	127.40
1	AA	1246	A	C8-N9-C4	6.48	108.39	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	84	A	C8-N9-C4	6.48	108.39	105.80
22	BA	480	A	C5-N7-C8	6.48	107.14	103.90
22	BA	730	A	C5-C6-N1	6.48	120.94	117.70
22	BA	1876	A	N3-C4-N9	6.48	132.58	127.40
1	AA	573	A	N3-C4-N9	6.48	132.58	127.40
1	AA	621	A	N3-C4-N9	6.48	132.58	127.40
22	BA	1028	A	C8-N9-C4	6.47	108.39	105.80
1	AA	452	A	N3-C4-N9	6.47	132.58	127.40
1	AA	655	A	N3-C4-N9	6.47	132.58	127.40
1	AA	759	A	C4-C5-N7	-6.47	107.46	110.70
22	BA	920	A	C5-N7-C8	6.47	107.14	103.90
1	AA	71	A	N9-C4-C5	6.47	108.39	105.80
22	BA	2761	A	N3-C4-N9	6.47	132.58	127.40
1	AA	408	A	C8-N9-C4	6.47	108.39	105.80
22	BA	917	A	C5-C6-N1	6.47	120.94	117.70
22	BA	2513	A	N3-C4-N9	6.47	132.57	127.40
23	BB	39	A	C4-C5-C6	6.47	120.23	117.00
22	BA	849	A	N3-C4-N9	6.47	132.57	127.40
22	BA	1919	A	C5-N7-C8	6.47	107.13	103.90
22	BA	2284	A	C4-C5-C6	6.47	120.23	117.00
22	BA	2850	A	N3-C4-N9	6.47	132.57	127.40
1	AA	338	A	C4-C5-C6	6.46	120.23	117.00
22	BA	609	A	C5-N7-C8	6.46	107.13	103.90
22	BA	1641	A	C4-C5-N7	-6.46	107.47	110.70
1	AA	152	A	N9-C4-C5	6.46	108.39	105.80
22	BA	2328	A	C5-N7-C8	6.46	107.13	103.90
22	BA	2868	A	C4-C5-C6	6.46	120.23	117.00
1	AA	66	A	C5-N7-C8	6.46	107.13	103.90
22	BA	195	A	N9-C4-C5	6.46	108.38	105.80
22	BA	756	A	C8-N9-C4	6.46	108.38	105.80
1	AA	155	A	C5-C6-N1	6.46	120.93	117.70
1	AA	171	A	C8-N9-C4	6.46	108.38	105.80
1	AA	1219	A	C5-N7-C8	6.46	107.13	103.90
22	BA	172	A	N3-C4-N9	6.46	132.57	127.40
22	BA	699	A	C4-C5-N7	-6.46	107.47	110.70
1	AA	51	A	C8-N9-C4	6.46	108.38	105.80
1	AA	1213	A	N9-C4-C5	6.46	108.38	105.80
1	AA	373	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1978	A	N3-C4-N9	6.45	132.56	127.40
23	BB	101	A	C6-N1-C2	-6.45	114.73	118.60
1	AA	174	A	N3-C4-N9	6.45	132.56	127.40
1	AA	1188	A	C4-C5-C6	6.45	120.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1191	A	N3-C4-N9	6.45	132.56	127.40
1	AA	1357	A	N9-C4-C5	6.45	108.38	105.80
22	BA	892	A	C4-C5-C6	6.45	120.22	117.00
22	BA	1000	A	C4-C5-C6	6.45	120.22	117.00
1	AA	414	A	N3-C4-N9	6.45	132.56	127.40
1	AA	1169	A	C8-N9-C4	6.45	108.38	105.80
22	BA	64	A	C8-N9-C4	6.45	108.38	105.80
22	BA	374	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1772	A	C8-N9-C4	6.45	108.38	105.80
22	BA	528	A	N9-C4-C5	6.44	108.38	105.80
22	BA	633	A	C4-C5-C6	6.44	120.22	117.00
22	BA	2749	A	C5-C6-N1	6.44	120.92	117.70
22	BA	532	A	N3-C4-N9	6.44	132.55	127.40
22	BA	1998	A	C4-C5-C6	6.44	120.22	117.00
1	AA	560	A	N3-C4-N9	6.44	132.55	127.40
22	BA	742	A	C5-C6-N1	6.44	120.92	117.70
22	BA	945	A	C4-C5-N7	-6.44	107.48	110.70
22	BA	1085	A	C4-C5-N7	-6.44	107.48	110.70
22	BA	1336	A	C8-N9-C4	6.44	108.38	105.80
22	BA	2450	A	C5-N7-C8	6.44	107.12	103.90
1	AA	192	A	C4-C5-C6	6.44	120.22	117.00
1	AA	630	A	N3-C4-N9	6.44	132.55	127.40
1	AA	1299	A	C4-C5-C6	6.44	120.22	117.00
22	BA	975	A	C5-N7-C8	6.44	107.12	103.90
22	BA	1308	A	C8-N9-C4	6.44	108.37	105.80
22	BA	2706	A	C4-C5-C6	6.44	120.22	117.00
22	BA	1502	A	C4-C5-C6	6.43	120.22	117.00
22	BA	1866	A	N3-C4-N9	6.43	132.55	127.40
22	BA	2117	A	C4-C5-C6	6.43	120.22	117.00
1	AA	787	A	C8-N9-C4	6.43	108.37	105.80
1	AA	864	A	C4-C5-C6	6.43	120.22	117.00
1	AA	69	G	C5-C6-N1	6.43	114.72	111.50
22	BA	1590	A	C4-C5-C6	6.43	120.22	117.00
1	AA	364	A	N9-C4-C5	6.43	108.37	105.80
1	AA	959	A	C4-C5-C6	6.43	120.21	117.00
1	AA	1180	A	C8-N9-C4	6.43	108.37	105.80
1	AA	1246	A	N3-C4-N9	6.43	132.54	127.40
1	AA	579	A	C4-C5-C6	6.43	120.21	117.00
1	AA	1360	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1088	A	C8-N9-C4	6.43	108.37	105.80
1	AA	459	A	N3-C4-N9	6.43	132.54	127.40
1	AA	509	A	N3-C4-N9	6.43	132.54	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1437	A	C4-C5-C6	6.43	120.21	117.00
22	BA	64	A	C5-C6-N1	6.43	120.91	117.70
22	BA	753	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1789	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1932	A	N3-C4-N9	6.43	132.54	127.40
1	AA	366	A	N3-C4-N9	6.42	132.54	127.40
1	AA	1130	A	C4-C5-C6	6.42	120.21	117.00
22	BA	322	A	N3-C4-N9	6.42	132.54	127.40
1	AA	1151	A	N3-C4-N9	6.42	132.54	127.40
22	BA	2147	A	C8-N9-C4	6.42	108.37	105.80
22	BA	2587	A	N3-C4-N9	6.42	132.54	127.40
1	AA	918	A	C8-N9-C4	6.42	108.37	105.80
22	BA	1392	A	C5-C6-N1	6.42	120.91	117.70
22	BA	1679	A	C5-N7-C8	6.42	107.11	103.90
22	BA	2482	A	C4-C5-C6	6.42	120.21	117.00
22	BA	2826	A	N3-C4-N9	6.42	132.54	127.40
22	BA	960	A	N3-C4-N9	6.42	132.53	127.40
22	BA	1260	A	C5-C6-N1	6.42	120.91	117.70
22	BA	1641	A	N9-C4-C5	6.42	108.37	105.80
22	BA	1678	A	C5-N7-C8	6.42	107.11	103.90
22	BA	2369	A	N3-C4-N9	6.42	132.53	127.40
22	BA	2665	A	N3-C4-N9	6.42	132.53	127.40
22	BA	1301	A	C8-N9-C4	6.42	108.37	105.80
22	BA	1977	A	N3-C4-N9	6.42	132.53	127.40
1	AA	482	A	N3-C4-N9	6.41	132.53	127.40
1	AA	695	A	N3-C4-N9	6.41	132.53	127.40
1	AA	1408	A	C4-C5-C6	6.41	120.21	117.00
22	BA	199	A	C5-C6-N1	6.41	120.91	117.70
22	BA	788	A	N3-C4-N9	6.41	132.53	127.40
22	BA	829	A	C5-N7-C8	6.41	107.11	103.90
22	BA	1237	A	C4-C5-C6	6.41	120.21	117.00
22	BA	1403	A	N9-C4-C5	6.41	108.36	105.80
22	BA	1593	A	N3-C4-N9	6.41	132.53	127.40
1	AA	478	A	C4-C5-C6	6.41	120.20	117.00
1	AA	831	A	C4-C5-C6	6.41	120.20	117.00
1	AA	845	A	N9-C4-C5	6.41	108.36	105.80
22	BA	346	A	C4-C5-C6	6.41	120.20	117.00
22	BA	2639	A	N3-C4-N9	6.41	132.53	127.40
22	BA	2662	A	N3-C4-N9	6.41	132.53	127.40
23	BB	53	A	N3-C4-N9	6.41	132.53	127.40
1	AA	815	A	N3-C4-N9	6.41	132.53	127.40
22	BA	1503	A	C4-C5-C6	6.41	120.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2829	A	C4-C5-N7	-6.41	107.50	110.70
23	BB	99	A	N9-C4-C5	6.41	108.36	105.80
1	AA	958	A	N9-C4-C5	6.41	108.36	105.80
22	BA	332	A	N9-C4-C5	6.41	108.36	105.80
22	BA	2814	A	C4-C5-C6	6.41	120.20	117.00
22	BA	655	A	N3-C4-N9	6.40	132.52	127.40
22	BA	2369	A	C5-C6-N1	6.40	120.90	117.70
1	AA	907	A	C8-N9-C4	6.40	108.36	105.80
22	BA	718	A	C8-N9-C4	6.40	108.36	105.80
22	BA	900	A	N3-C4-N9	6.40	132.52	127.40
22	BA	1040	A	C8-N9-C4	6.40	108.36	105.80
22	BA	1069	A	C4-C5-N7	-6.40	107.50	110.70
1	AA	547	A	C4-C5-N7	-6.40	107.50	110.70
1	AA	1271	A	C8-N9-C4	6.40	108.36	105.80
22	BA	715	A	C4-C5-C6	6.40	120.20	117.00
1	AA	7	A	N9-C4-C5	6.40	108.36	105.80
1	AA	139	A	N3-C4-N9	6.40	132.52	127.40
22	BA	347	A	C4-C5-C6	6.40	120.20	117.00
22	BA	2534	A	C4-C5-C6	6.40	120.20	117.00
55	B8	41	A	N3-C4-N9	6.40	132.52	127.40
22	BA	103	A	C8-N9-C4	6.39	108.36	105.80
22	BA	221	A	C5-N7-C8	6.39	107.10	103.90
22	BA	2542	A	C5-C6-N1	6.39	120.90	117.70
1	AA	151	A	N3-C4-N9	6.39	132.51	127.40
1	AA	1493	A	N3-C4-N9	6.39	132.51	127.40
22	BA	1321	A	N3-C4-N9	6.39	132.51	127.40
22	BA	1960	A	C4-C5-C6	6.39	120.20	117.00
22	BA	1829	A	C4-C5-N7	-6.39	107.50	110.70
22	BA	911	A	C5-N7-C8	6.39	107.09	103.90
22	BA	1590	A	C5-C6-N1	6.39	120.89	117.70
22	BA	2158	A	C4-C5-C6	6.39	120.19	117.00
1	AA	495	A	C4-C5-C6	6.39	120.19	117.00
1	AA	1289	A	C8-N9-C4	6.39	108.36	105.80
1	AA	1429	A	N3-C4-N9	6.39	132.51	127.40
22	BA	449	A	C4-C5-C6	6.39	120.19	117.00
22	BA	2314	A	C4-C5-C6	6.39	120.19	117.00
23	BB	57	A	N3-C4-N9	6.39	132.51	127.40
1	AA	560	A	C4-C5-C6	6.39	120.19	117.00
22	BA	2736	A	N3-C4-N9	6.39	132.51	127.40
1	AA	67	C	C6-N1-C2	6.38	122.85	120.30
22	BA	478	A	C5-N7-C8	6.38	107.09	103.90
22	BA	1597	A	C4-C5-C6	6.38	120.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2471	A	C5-C6-N1	6.38	120.89	117.70
22	BA	2800	A	C4-C5-N7	-6.38	107.51	110.70
23	BB	58	A	N3-C4-N9	6.38	132.51	127.40
22	BA	1553	A	C8-N9-C4	6.38	108.35	105.80
1	AA	448	A	C4-C5-C6	6.38	120.19	117.00
22	BA	2448	A	N3-C4-N9	6.38	132.50	127.40
22	BA	384	A	N3-C4-N9	6.38	132.50	127.40
1	AA	353	A	N3-C4-N9	6.38	132.50	127.40
22	BA	721	A	N3-C4-N9	6.38	132.50	127.40
22	BA	1544	A	C4-C5-C6	6.38	120.19	117.00
23	BB	58	A	C4-C5-N7	-6.38	107.51	110.70
1	AA	116	A	C5-N7-C8	6.38	107.09	103.90
22	BA	197	A	C4-C5-C6	6.38	120.19	117.00
22	BA	794	A	N3-C4-N9	6.38	132.50	127.40
22	BA	945	A	N3-C4-N9	6.38	132.50	127.40
22	BA	1321	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1698	A	C8-N9-C4	6.38	108.35	105.80
22	BA	2378	A	C5-N7-C8	6.38	107.09	103.90
1	AA	315	A	C4-C5-C6	6.38	120.19	117.00
22	BA	877	A	C5-C6-N1	6.38	120.89	117.70
22	BA	10	A	C8-N9-C4	6.37	108.35	105.80
22	BA	470	A	N3-C4-N9	6.37	132.50	127.40
22	BA	1808	A	C8-N9-C4	6.37	108.35	105.80
22	BA	2352	A	C4-C5-C6	6.37	120.19	117.00
22	BA	2711	A	C8-N9-C4	6.37	108.35	105.80
23	BB	53	A	C4-C5-C6	6.37	120.19	117.00
22	BA	899	A	N3-C4-N9	6.37	132.50	127.40
22	BA	2725	A	C5-C6-N1	6.37	120.89	117.70
1	AA	59	A	C8-N9-C4	6.37	108.35	105.80
22	BA	959	A	N3-C4-N9	6.37	132.50	127.40
22	BA	1373	A	C4-C5-C6	6.37	120.19	117.00
1	AA	1398	A	C8-N9-C4	6.37	108.35	105.80
22	BA	603	A	C4-C5-C6	6.37	120.18	117.00
22	BA	1144	A	C4-C5-C6	6.37	120.18	117.00
22	BA	1366	A	C5-N7-C8	6.37	107.08	103.90
23	BB	34	A	N9-C4-C5	6.37	108.35	105.80
1	AA	72	A	C4-C5-C6	6.37	120.18	117.00
1	AA	1430	A	C5-N7-C8	6.37	107.08	103.90
22	BA	1744	A	N9-C4-C5	6.37	108.35	105.80
1	AA	182	A	N3-C4-N9	6.37	132.49	127.40
1	AA	1229	A	C4-C5-C6	6.37	120.18	117.00
22	BA	644	A	C8-N9-C4	6.37	108.35	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2082	A	N3-C4-N9	6.37	132.49	127.40
1	AA	33	A	C4-C5-C6	6.36	120.18	117.00
1	AA	459	A	C5-C6-N1	6.36	120.88	117.70
22	BA	118	A	N3-C4-N9	6.36	132.49	127.40
22	BA	342	A	C8-N9-C4	6.36	108.34	105.80
22	BA	599	A	N9-C4-C5	6.36	108.34	105.80
22	BA	1668	A	C4-C5-N7	-6.36	107.52	110.70
22	BA	2298	A	N3-C4-N9	6.36	132.49	127.40
1	AA	1082	A	N3-C4-N9	6.36	132.49	127.40
22	BA	1367	A	C4-C5-C6	6.36	120.18	117.00
22	BA	1665	A	C5-C6-N1	6.36	120.88	117.70
22	BA	2501	C	C2-N1-C1'	-6.36	111.80	118.80
1	AA	374	A	C4-C5-C6	6.36	120.18	117.00
22	BA	933	A	C4-C5-N7	-6.36	107.52	110.70
22	BA	963	U	O5'-P-OP1	-6.36	99.97	105.70
22	BA	1151	A	C4-C5-C6	6.36	120.18	117.00
22	BA	1264	A	C5-N7-C8	6.36	107.08	103.90
1	AA	1493	A	C8-N9-C4	6.36	108.34	105.80
22	BA	1927	A	N9-C4-C5	6.36	108.34	105.80
1	AA	968	A	N3-C4-N9	6.36	132.49	127.40
22	BA	64	A	C4-C5-C6	6.36	120.18	117.00
22	BA	661	A	C4-C5-N7	-6.36	107.52	110.70
22	BA	1103	A	N3-C4-N9	6.36	132.49	127.40
22	BA	2598	A	N3-C4-N9	6.36	132.48	127.40
1	AA	130	A	C4-C5-C6	6.35	120.18	117.00
22	BA	503	A	C5-C6-N1	6.35	120.88	117.70
1	AA	468	A	N3-C4-N9	6.35	132.48	127.40
1	AA	978	A	N9-C4-C5	6.35	108.34	105.80
1	AA	1016	A	C4-C5-N7	-6.35	107.52	110.70
1	AA	1429	A	C4-C5-C6	6.35	120.18	117.00
22	BA	1246	A	C5-C6-N1	6.35	120.88	117.70
22	BA	1395	A	N9-C4-C5	6.35	108.34	105.80
22	BA	1654	A	N3-C4-N9	6.35	132.48	127.40
22	BA	2518	A	C5-C6-N1	6.35	120.88	117.70
1	AA	59	A	N3-C4-N9	6.35	132.48	127.40
1	AA	60	A	C4-C5-N7	-6.35	107.52	110.70
1	AA	815	A	C8-N9-C4	6.35	108.34	105.80
1	AA	865	A	N9-C4-C5	6.35	108.34	105.80
1	AA	228	A	N3-C4-N9	6.35	132.48	127.40
1	AA	466	A	N3-C4-N9	6.35	132.48	127.40
1	AA	1022	A	C8-N9-C4	6.35	108.34	105.80
1	AA	1252	A	C8-N9-C4	6.35	108.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1308	A	C4-C5-C6	6.35	120.17	117.00
22	BA	1866	A	C4-C5-C6	6.35	120.17	117.00
22	BA	2154	A	C4-C5-N7	-6.35	107.53	110.70
55	B8	26	A	N3-C4-N9	6.35	132.48	127.40
1	AA	918	A	C4-C5-N7	-6.35	107.53	110.70
1	AA	1433	A	N3-C4-N9	6.35	132.48	127.40
22	BA	74	A	C8-N9-C4	6.35	108.34	105.80
22	BA	222	A	N3-C4-N9	6.35	132.48	127.40
22	BA	2634	A	C4-C5-C6	6.35	120.17	117.00
22	BA	2635	A	N3-C4-N9	6.35	132.48	127.40
1	AA	676	A	C4-C5-C6	6.35	120.17	117.00
1	AA	1227	A	C4-C5-C6	6.35	120.17	117.00
1	AA	909	A	C4-C5-C6	6.34	120.17	117.00
1	AA	935	A	N3-C4-N9	6.34	132.48	127.40
1	AA	937	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1197	A	C8-N9-C4	6.34	108.34	105.80
22	BA	866	A	N3-C4-N9	6.34	132.48	127.40
22	BA	1029	A	C8-N9-C4	6.34	108.34	105.80
22	BA	1169	A	C8-N9-C4	6.34	108.34	105.80
22	BA	1637	A	N3-C4-N9	6.34	132.48	127.40
22	BA	2893	A	N3-C4-N9	6.34	132.48	127.40
1	AA	914	A	C8-N9-C4	6.34	108.34	105.80
1	AA	1171	A	C5-C6-N1	6.34	120.87	117.70
1	AA	539	A	C4-C5-C6	6.34	120.17	117.00
1	AA	937	A	C8-N9-C4	6.34	108.34	105.80
22	BA	2700	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1157	A	N9-C4-C5	6.34	108.34	105.80
22	BA	457	A	C5-C6-N1	6.34	120.87	117.70
22	BA	716	A	C8-N9-C4	6.34	108.34	105.80
22	BA	1970	A	C8-N9-C4	6.34	108.33	105.80
1	AA	1493	A	C4-C5-C6	6.34	120.17	117.00
22	BA	2856	A	C4-C5-N7	-6.34	107.53	110.70
1	AA	253	A	C4-C5-C6	6.34	120.17	117.00
22	BA	1889	A	C5-C6-N1	6.34	120.87	117.70
1	AA	161	A	C4-C5-C6	6.33	120.17	117.00
1	AA	704	A	C5-N7-C8	6.33	107.07	103.90
22	BA	5	A	C5-C6-N1	6.33	120.87	117.70
22	BA	1853	A	C8-N9-C4	6.33	108.33	105.80
1	AA	1000	A	C8-N9-C4	6.33	108.33	105.80
22	BA	219	A	C4-C5-C6	6.33	120.17	117.00
22	BA	1039	A	N3-C4-N9	6.33	132.47	127.40
22	BA	2071	A	C5-N7-C8	6.33	107.07	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2267	A	C5-C6-N1	6.33	120.86	117.70
22	BA	2333	A	N3-C4-N9	6.33	132.46	127.40
22	BA	126	A	C4-C5-N7	-6.33	107.54	110.70
22	BA	2101	A	N9-C4-C5	6.33	108.33	105.80
22	BA	2516	A	N9-C4-C5	6.33	108.33	105.80
22	BA	2873	A	N3-C4-N9	6.33	132.46	127.40
23	BB	15	A	C5-N7-C8	6.33	107.06	103.90
22	BA	1308	A	N9-C4-C5	6.33	108.33	105.80
22	BA	2518	A	C4-C5-C6	6.33	120.16	117.00
1	AA	431	A	N9-C4-C5	6.32	108.33	105.80
22	BA	272	A	C8-N9-C4	6.32	108.33	105.80
22	BA	637	A	C8-N9-C4	6.32	108.33	105.80
22	BA	1913	A	N3-C4-N9	6.32	132.46	127.40
22	BA	2088	A	C8-N9-C4	6.32	108.33	105.80
22	BA	2447	G	N3-C4-C5	-6.32	125.44	128.60
1	AA	1080	A	N3-C4-N9	6.32	132.46	127.40
22	BA	481	G	O4'-C1'-N9	6.32	113.26	108.20
22	BA	2748	A	C5-C6-N1	6.32	120.86	117.70
1	AA	69	G	C1'-O4'-C4'	-6.32	104.84	109.90
1	AA	363	A	C4-C5-N7	-6.32	107.54	110.70
1	AA	553	A	C8-N9-C4	6.32	108.33	105.80
1	AA	609	A	C8-N9-C4	6.32	108.33	105.80
1	AA	1441	A	C4-C5-C6	6.32	120.16	117.00
1	AA	1446	A	N9-C4-C5	6.32	108.33	105.80
22	BA	255	A	N3-C4-N9	6.32	132.46	127.40
22	BA	262	A	C5-C6-N1	6.32	120.86	117.70
22	BA	1749	A	C5-C6-N1	6.32	120.86	117.70
22	BA	1871	A	N3-C4-N9	6.32	132.46	127.40
22	BA	1900	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2516	A	C5-C6-N1	6.32	120.86	117.70
22	BA	905	A	N3-C4-N9	6.32	132.45	127.40
22	BA	1848	A	N3-C4-N9	6.32	132.46	127.40
22	BA	2088	A	C5-C6-N1	6.32	120.86	117.70
1	AA	51	A	C4-C5-C6	6.32	120.16	117.00
22	BA	1427	A	C8-N9-C4	6.32	108.33	105.80
22	BA	1784	A	N3-C4-N9	6.32	132.45	127.40
22	BA	1069	A	N3-C4-N9	6.31	132.45	127.40
1	AA	1257	A	C4-C5-C6	6.31	120.16	117.00
22	BA	28	A	N3-C4-N9	6.31	132.45	127.40
22	BA	2003	A	N3-C4-N9	6.31	132.45	127.40
23	BB	101	A	N9-C4-C5	6.31	108.33	105.80
1	AA	1306	A	N3-C4-N9	6.31	132.45	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1433	A	C8-N9-C4	6.31	108.32	105.80
22	BA	217	A	C5-N7-C8	6.31	107.06	103.90
1	AA	1012	A	C4-C5-C6	6.31	120.15	117.00
22	BA	1070	A	C4-C5-C6	6.31	120.15	117.00
1	AA	72	A	N3-C4-N9	6.30	132.44	127.40
1	AA	1433	A	C5-C6-N1	6.30	120.85	117.70
22	BA	603	A	C8-N9-C4	6.30	108.32	105.80
22	BA	1378	A	C4-C5-N7	-6.30	107.55	110.70
22	BA	2634	A	C8-N9-C4	6.30	108.32	105.80
22	BA	2829	A	N3-C4-N9	6.30	132.44	127.40
1	AA	101	A	N9-C4-C5	6.30	108.32	105.80
22	BA	244	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1821	A	C8-N9-C4	6.30	108.32	105.80
22	BA	2169	A	C4-C5-C6	6.30	120.15	117.00
22	BA	2198	A	C4-C5-C6	6.30	120.15	117.00
22	BA	2531	A	C8-N9-C4	6.30	108.32	105.80
23	BB	99	A	C4-C5-N7	-6.30	107.55	110.70
1	AA	676	A	N3-C4-N9	6.30	132.44	127.40
22	BA	1001	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1111	A	C8-N9-C4	6.30	108.32	105.80
22	BA	1755	A	C4-C5-N7	-6.30	107.55	110.70
22	BA	2186	G	C5-C6-O6	6.30	132.38	128.60
1	AA	117	G	O5'-P-OP2	6.30	118.26	110.70
1	AA	596	A	C4-C5-C6	6.30	120.15	117.00
1	AA	1110	A	C4-C5-C6	6.30	120.15	117.00
1	AA	1431	A	C8-N9-C4	6.30	108.32	105.80
22	BA	449	A	C8-N9-C4	6.30	108.32	105.80
22	BA	1077	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1029	A	C4-C5-C6	6.29	120.15	117.00
22	BA	2317	A	C5-C6-N1	6.29	120.85	117.70
1	AA	321	A	C5-C6-N1	6.29	120.85	117.70
1	AA	728	A	N3-C4-N9	6.29	132.44	127.40
22	BA	156	A	C4-C5-C6	6.29	120.15	117.00
22	BA	1272	A	N3-C4-N9	6.29	132.44	127.40
22	BA	71	A	N3-C4-N9	6.29	132.43	127.40
22	BA	374	A	C8-N9-C4	6.29	108.32	105.80
22	BA	905	A	C8-N9-C4	6.29	108.32	105.80
22	BA	1551	A	N3-C4-N9	6.29	132.43	127.40
1	AA	1012	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1515	A	C4-C5-N7	-6.29	107.56	110.70
22	BA	1572	A	C5-C6-N1	6.29	120.84	117.70
22	BA	1953	A	N3-C4-N9	6.29	132.43	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2434	A	N3-C4-N9	6.29	132.43	127.40
22	BA	2682	A	C5-C6-N1	6.29	120.84	117.70
1	AA	109	A	C4-C5-C6	6.29	120.14	117.00
1	AA	482	A	C4-C5-C6	6.29	120.14	117.00
1	AA	542	G	O4'-C1'-N9	6.29	113.23	108.20
1	AA	1250	A	C4-C5-C6	6.29	120.14	117.00
22	BA	49	A	N3-C4-N9	6.29	132.43	127.40
22	BA	56	A	C5-C6-N1	6.29	120.84	117.70
22	BA	1265	A	C5-C6-N1	6.29	120.84	117.70
1	AA	74	A	C4-C5-C6	6.28	120.14	117.00
22	BA	460	A	N3-C4-N9	6.28	132.43	127.40
22	BA	466	A	N3-C4-N9	6.28	132.43	127.40
22	BA	497	A	N3-C4-N9	6.28	132.43	127.40
22	BA	2366	A	N3-C4-N9	6.28	132.43	127.40
22	BA	2426	A	C5-N7-C8	6.28	107.04	103.90
22	BA	2781	A	N3-C4-N9	6.28	132.43	127.40
22	BA	1103	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1634	A	N3-C4-N9	6.28	132.43	127.40
22	BA	1786	A	N3-C4-N9	6.28	132.43	127.40
22	BA	371	A	C5-C6-N1	6.28	120.84	117.70
22	BA	2070	A	C4-C5-C6	6.28	120.14	117.00
22	BA	2406	A	C8-N9-C4	6.28	108.31	105.80
22	BA	111	A	C8-N9-C4	6.28	108.31	105.80
22	BA	199	A	N9-C4-C5	6.28	108.31	105.80
1	AA	246	A	N9-C4-C5	6.28	108.31	105.80
1	AA	553	A	C4-C5-C6	6.28	120.14	117.00
1	AA	523	A	C8-N9-C4	6.28	108.31	105.80
22	BA	526	A	N3-C4-N9	6.28	132.42	127.40
22	BA	1247	A	C8-N9-C4	6.28	108.31	105.80
1	AA	747	A	N3-C4-N9	6.27	132.42	127.40
22	BA	2346	A	C4-C5-C6	6.27	120.14	117.00
1	AA	900	A	C5-C6-N1	6.27	120.84	117.70
22	BA	1490	A	C8-N9-C4	6.27	108.31	105.80
22	BA	1762	A	C5-N7-C8	6.27	107.04	103.90
22	BA	2051	A	C5-C6-N1	6.27	120.84	117.70
22	BA	2070	A	C4-C5-N7	-6.27	107.56	110.70
22	BA	2711	A	C5-N7-C8	6.27	107.04	103.90
1	AA	415	A	N3-C4-N9	6.27	132.42	127.40
22	BA	21	A	C5-C6-N1	6.27	120.83	117.70
22	BA	1616	A	N3-C4-N9	6.27	132.41	127.40
22	BA	2225	A	C8-N9-C4	6.27	108.31	105.80
22	BA	2682	A	C5-N7-C8	6.27	107.03	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	59	A	N3-C4-N9	6.27	132.41	127.40
1	AA	364	A	C4-C5-C6	6.27	120.13	117.00
22	BA	2476	A	N9-C4-C5	6.27	108.31	105.80
1	AA	441	A	C4-C5-C6	6.26	120.13	117.00
22	BA	1169	A	C4-C5-C6	6.26	120.13	117.00
22	BA	322	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2031	A	N3-C4-N9	6.26	132.41	127.40
1	AA	303	A	C8-N9-C4	6.26	108.30	105.80
1	AA	315	A	N9-C4-C5	6.26	108.31	105.80
22	BA	83	A	N3-C4-N9	6.26	132.41	127.40
22	BA	423	A	N9-C4-C5	6.26	108.31	105.80
22	BA	1477	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2425	A	N3-C4-N9	6.26	132.41	127.40
1	AA	563	A	C4-C5-C6	6.26	120.13	117.00
22	BA	990	A	N3-C4-N9	6.26	132.41	127.40
1	AA	909	A	N9-C4-C5	6.26	108.30	105.80
22	BA	925	A	C8-N9-C4	6.26	108.30	105.80
22	BA	1969	A	N3-C4-N9	6.26	132.41	127.40
1	AA	172	A	C8-N9-C4	6.26	108.30	105.80
1	AA	327	A	C5-C6-N1	6.26	120.83	117.70
1	AA	572	A	C4-C5-N7	-6.26	107.57	110.70
22	BA	820	A	C5-N7-C8	6.26	107.03	103.90
22	BA	2501	C	C6-N1-C1'	6.26	128.31	120.80
1	AA	149	A	C4-C5-N7	-6.25	107.57	110.70
22	BA	718	A	C4-C5-C6	6.25	120.13	117.00
22	BA	2322	A	C8-N9-C4	6.25	108.30	105.80
1	AA	205	A	C4-C5-C6	6.25	120.13	117.00
22	BA	362	A	C8-N9-C4	6.25	108.30	105.80
22	BA	743	A	C8-N9-C4	6.25	108.30	105.80
22	BA	1496	A	C4-C5-C6	6.25	120.13	117.00
1	AA	461	A	N9-C4-C5	6.25	108.30	105.80
1	AA	563	A	C4-C5-N7	-6.25	107.57	110.70
1	AA	1188	A	C8-N9-C4	6.25	108.30	105.80
1	AA	1350	A	N3-C4-N9	6.25	132.40	127.40
22	BA	501	A	C4-C5-C6	6.25	120.13	117.00
22	BA	1074	G	N1-C6-O6	-6.25	116.15	119.90
22	BA	2572	A	C8-N9-C4	6.25	108.30	105.80
22	BA	2119	A	C4-C5-N7	-6.25	107.58	110.70
22	BA	2518	A	C8-N9-C4	6.25	108.30	105.80
1	AA	579	A	N3-C4-N9	6.25	132.40	127.40
1	AA	49	U	C5-C4-O4	6.25	129.65	125.90
1	AA	288	A	C4-C5-C6	6.25	120.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	743	A	C8-N9-C4	6.25	108.30	105.80
1	AA	860	A	N3-C4-N9	6.25	132.40	127.40
22	BA	449	A	C5-C6-N1	6.25	120.82	117.70
1	AA	767	A	C4-C5-C6	6.25	120.12	117.00
22	BA	89	A	C8-N9-C4	6.25	108.30	105.80
22	BA	272	A	C4-C5-C6	6.25	120.12	117.00
1	AA	179	A	N9-C4-C5	6.24	108.30	105.80
1	AA	448	A	N3-C4-N9	6.24	132.40	127.40
22	BA	71	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1085	A	N3-C4-N9	6.24	132.40	127.40
22	BA	1759	A	C8-N9-C4	6.24	108.30	105.80
22	BA	2733	A	N3-C4-N9	6.24	132.39	127.40
1	AA	152	A	C4-C5-N7	-6.24	107.58	110.70
1	AA	192	A	C5-C6-N1	6.24	120.82	117.70
1	AA	451	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1216	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1679	A	C4-C5-C6	6.24	120.12	117.00
22	BA	272	A	N3-C4-N9	6.24	132.39	127.40
22	BA	330	A	C4-C5-C6	6.24	120.12	117.00
22	BA	727	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1689	A	N3-C4-N9	6.24	132.39	127.40
22	BA	2135	A	C4-C5-C6	6.24	120.12	117.00
22	BA	2298	A	C4-C5-C6	6.24	120.12	117.00
22	BA	2757	A	C5-N7-C8	6.24	107.02	103.90
22	BA	1912	A	N9-C4-C5	6.24	108.30	105.80
1	AA	1155	A	C8-N9-C4	6.24	108.30	105.80
1	AA	435	A	N3-C4-N9	6.24	132.39	127.40
1	AA	1197	A	N3-C4-N9	6.24	132.39	127.40
22	BA	492	A	N3-C4-N9	6.24	132.39	127.40
22	BA	1155	A	N9-C4-C5	6.24	108.29	105.80
22	BA	2176	A	C8-N9-C4	6.24	108.29	105.80
1	AA	790	A	C4-C5-C6	6.23	120.12	117.00
22	BA	156	A	C8-N9-C4	6.23	108.29	105.80
23	BB	50	A	C8-N9-C4	6.23	108.29	105.80
1	AA	321	A	C4-C5-C6	6.23	120.11	117.00
1	AA	712	A	C5-C6-N1	6.23	120.81	117.70
22	BA	223	A	C8-N9-C4	6.23	108.29	105.80
22	BA	2212	A	C4-C5-C6	6.23	120.11	117.00
22	BA	513	A	C8-N9-C4	6.23	108.29	105.80
22	BA	984	A	N3-C4-N9	6.23	132.38	127.40
22	BA	1393	A	C4-C5-C6	6.23	120.11	117.00
22	BA	2826	A	C5-C6-N1	6.23	120.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1403	A	C4-C5-C6	6.23	120.11	117.00
22	BA	1858	A	N3-C4-N9	6.23	132.38	127.40
22	BA	2340	A	C5-C6-N1	6.23	120.81	117.70
1	AA	28	A	N3-C4-N9	6.22	132.38	127.40
1	AA	553	A	N3-C4-N9	6.22	132.38	127.40
22	BA	53	A	C8-N9-C4	6.22	108.29	105.80
1	AA	642	A	N3-C4-N9	6.22	132.38	127.40
1	AA	1476	A	C8-N9-C4	6.22	108.29	105.80
22	BA	1095	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1111	A	N3-C4-N9	6.22	132.38	127.40
22	BA	2267	A	C4-C5-N7	-6.22	107.59	110.70
54	B7	9	A	N9-C4-C5	6.22	108.29	105.80
22	BA	2311	A	N9-C4-C5	6.22	108.29	105.80
1	AA	782	A	C5-N7-C8	6.22	107.01	103.90
1	AA	864	A	N3-C4-N9	6.22	132.38	127.40
22	BA	310	A	C5-C6-N1	6.22	120.81	117.70
55	B8	14	A	C4-C5-C6	6.22	120.11	117.00
22	BA	125	A	C8-N9-C4	6.22	108.29	105.80
22	BA	1652	A	C4-C5-N7	-6.22	107.59	110.70
22	BA	2013	A	C4-C5-C6	6.22	120.11	117.00
1	AA	1236	A	C8-N9-C4	6.22	108.29	105.80
22	BA	504	A	C4-C5-C6	6.22	120.11	117.00
22	BA	1632	A	C8-N9-C4	6.22	108.29	105.80
22	BA	2856	A	N9-C4-C5	6.22	108.29	105.80
54	B7	9	A	C4-C5-N7	-6.22	107.59	110.70
22	BA	899	A	C4-C5-C6	6.21	120.11	117.00
1	AA	959	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1610	A	C5-C6-N1	6.21	120.81	117.70
1	AA	595	A	C4-C5-C6	6.21	120.11	117.00
1	AA	974	A	N3-C4-N9	6.21	132.37	127.40
1	AA	1093	A	C4-C5-C6	6.21	120.11	117.00
22	BA	38	A	N9-C4-C5	6.21	108.28	105.80
22	BA	53	A	C5-C6-N1	6.21	120.81	117.70
22	BA	2173	A	C8-N9-C4	6.21	108.28	105.80
22	BA	1952	A	C4-C5-C6	6.21	120.11	117.00
1	AA	900	A	N3-C4-N9	6.21	132.37	127.40
22	BA	241	A	C5-N7-C8	6.21	107.00	103.90
22	BA	722	A	C4-C5-C6	6.21	120.10	117.00
22	BA	2435	A	C4-C5-C6	6.21	120.11	117.00
1	AA	238	A	C4-C5-N7	-6.21	107.60	110.70
1	AA	978	A	C4-C5-C6	6.21	120.10	117.00
22	BA	213	A	N3-C4-N9	6.21	132.37	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	415	A	C5-C6-N1	6.21	120.80	117.70
22	BA	2366	A	C5-N7-C8	6.21	107.00	103.90
1	AA	1394	A	C4-C5-C6	6.21	120.10	117.00
22	BA	1244	A	C4-C5-N7	-6.20	107.60	110.70
22	BA	2327	A	C4-C5-N7	-6.20	107.60	110.70
1	AA	539	A	C5-C6-N1	6.20	120.80	117.70
22	BA	614	A	C4-C5-C6	6.20	120.10	117.00
22	BA	749	A	N3-C4-N9	6.20	132.36	127.40
1	AA	66	A	C4-C5-C6	6.20	120.10	117.00
22	BA	753	A	C5-C6-N1	6.20	120.80	117.70
1	AA	44	A	C4-C5-N7	-6.20	107.60	110.70
1	AA	349	A	C8-N9-C4	6.20	108.28	105.80
22	BA	1347	A	C5-N7-C8	6.20	107.00	103.90
22	BA	575	A	C8-N9-C4	6.20	108.28	105.80
22	BA	900	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1280	A	N3-C4-N9	6.19	132.35	127.40
22	BA	827	U	OP1-P-OP2	6.19	128.89	119.60
22	BA	1040	A	C5-C6-N1	6.19	120.80	117.70
55	B8	58	A	C8-N9-C4	6.19	108.28	105.80
22	BA	6	A	N9-C4-C5	6.19	108.28	105.80
22	BA	1134	A	C5-C6-N1	6.19	120.80	117.70
22	BA	1650	A	N3-C4-N9	6.19	132.35	127.40
1	AA	1446	A	C4-C5-C6	6.19	120.10	117.00
22	BA	863	A	C5-C6-N1	6.19	120.80	117.70
22	BA	1169	A	N3-C4-N9	6.19	132.35	127.40
22	BA	2020	A	N3-C4-N9	6.19	132.35	127.40
1	AA	1044	A	N3-C4-N9	6.19	132.35	127.40
22	BA	300	A	N3-C4-N9	6.19	132.35	127.40
22	BA	310	A	C8-N9-C4	6.19	108.28	105.80
1	AA	10	A	N3-C4-N9	6.18	132.35	127.40
1	AA	1014	A	C4-C5-C6	6.18	120.09	117.00
22	BA	429	A	C4-C5-C6	6.18	120.09	117.00
22	BA	782	A	N3-C4-N9	6.18	132.35	127.40
22	BA	2758	A	N3-C4-N9	6.18	132.35	127.40
1	AA	1044	A	C4-C5-C6	6.18	120.09	117.00
22	BA	2327	A	N3-C4-N9	6.18	132.35	127.40
22	BA	2471	A	N9-C4-C5	6.18	108.27	105.80
1	AA	50	A	N3-C4-N9	6.18	132.34	127.40
22	BA	1084	A	N9-C4-C5	6.18	108.27	105.80
1	AA	974	A	C4-C5-C6	6.18	120.09	117.00
22	BA	1504	A	N3-C4-N9	6.18	132.34	127.40
22	BA	1548	A	C8-N9-C4	6.18	108.27	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	596	A	N3-C4-N9	6.18	132.34	127.40
1	AA	1145	A	N9-C4-C5	6.18	108.27	105.80
1	AA	1251	A	C4-C5-N7	-6.18	107.61	110.70
22	BA	693	A	C4-C5-N7	-6.18	107.61	110.70
22	BA	1010	A	C8-N9-C4	6.18	108.27	105.80
22	BA	2407	A	C8-N9-C4	6.18	108.27	105.80
22	BA	1155	A	C4-C5-N7	-6.18	107.61	110.70
22	BA	1586	A	N9-C4-C5	6.18	108.27	105.80
22	BA	216	A	C8-N9-C4	6.17	108.27	105.80
22	BA	1579	A	C4-C5-C6	6.17	120.09	117.00
22	BA	1899	A	N3-C4-N9	6.17	132.34	127.40
1	AA	790	A	N3-C4-N9	6.17	132.34	127.40
22	BA	532	A	C4-C5-C6	6.17	120.09	117.00
1	AA	523	A	N3-C4-N9	6.17	132.34	127.40
1	AA	914	A	N3-C4-N9	6.17	132.34	127.40
22	BA	6	A	C5-C6-N1	6.17	120.78	117.70
22	BA	750	A	C5-C6-N1	6.17	120.79	117.70
22	BA	1735	A	C8-N9-C4	6.17	108.27	105.80
22	BA	706	A	N9-C4-C5	6.17	108.27	105.80
22	BA	1050	A	N3-C4-N9	6.17	132.34	127.40
22	BA	1579	A	N3-C4-N9	6.17	132.34	127.40
22	BA	1786	A	N9-C4-C5	6.17	108.27	105.80
1	AA	946	A	C8-N9-C4	6.17	108.27	105.80
1	AA	994	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1004	A	N3-C4-N9	6.17	132.33	127.40
22	BA	204	A	N9-C4-C5	6.17	108.27	105.80
22	BA	457	A	C8-N9-C4	6.17	108.27	105.80
22	BA	2186	G	N1-C6-O6	-6.17	116.20	119.90
22	BA	2211	A	N3-C4-N9	6.17	132.34	127.40
22	BA	541	A	C4-C5-N7	-6.17	107.62	110.70
22	BA	2829	A	C5-C6-N1	6.17	120.78	117.70
23	BB	29	A	N9-C4-C5	6.17	108.27	105.80
1	AA	66	A	C5-C6-N1	6.17	120.78	117.70
22	BA	1127	A	N3-C4-N9	6.17	132.33	127.40
22	BA	1549	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2706	A	N3-C4-N9	6.17	132.33	127.40
1	AA	196	A	N3-C4-N9	6.16	132.33	127.40
22	BA	422	A	C5-N7-C8	6.16	106.98	103.90
22	BA	1698	A	C4-C5-C6	6.16	120.08	117.00
22	BA	2314	A	N9-C4-C5	6.16	108.27	105.80
23	BB	52	A	C8-N9-C4	6.16	108.27	105.80
22	BA	422	A	C4-C5-C6	6.16	120.08	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	877	A	C4-C5-C6	6.16	120.08	117.00
1	AA	1042	A	N9-C4-C5	6.16	108.26	105.80
22	BA	909	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1010	A	C5-N7-C8	6.16	106.98	103.90
22	BA	1698	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1900	A	C8-N9-C4	6.16	108.26	105.80
23	BB	58	A	N9-C4-C5	6.16	108.26	105.80
1	AA	621	A	C8-N9-C4	6.16	108.26	105.80
22	BA	221	A	C4-C5-C6	6.16	120.08	117.00
22	BA	2095	A	N3-C4-N9	6.16	132.32	127.40
55	B8	14	A	N3-C4-N9	6.16	132.32	127.40
1	AA	790	A	C5-N7-C8	6.15	106.98	103.90
22	BA	1876	A	C5-C6-N1	6.15	120.78	117.70
22	BA	2748	A	C5-N7-C8	6.15	106.98	103.90
1	AA	28	A	C5-C6-N1	6.15	120.78	117.70
1	AA	172	A	C4-C5-C6	6.15	120.08	117.00
1	AA	498	A	C5-C6-N6	6.15	128.62	123.70
1	AA	1360	A	C8-N9-C4	6.15	108.26	105.80
1	AA	1500	A	C8-N9-C4	6.15	108.26	105.80
22	BA	454	A	C4-C5-C6	6.15	120.08	117.00
22	BA	783	A	C4-C5-C6	6.15	120.08	117.00
23	BB	75	G	C5-C6-N1	6.15	114.58	111.50
55	B8	66	A	C4-C5-C6	6.15	120.08	117.00
1	AA	520	A	C4-C5-C6	6.15	120.08	117.00
22	BA	142	A	N3-C4-N9	6.15	132.32	127.40
22	BA	256	A	C8-N9-C4	6.15	108.26	105.80
22	BA	633	A	C5-N7-C8	6.15	106.98	103.90
22	BA	910	A	N3-C4-N9	6.15	132.32	127.40
22	BA	1664	A	O5'-P-OP1	-6.15	100.17	105.70
22	BA	2278	A	N9-C4-C5	6.15	108.26	105.80
1	AA	262	A	C8-N9-C4	6.15	108.26	105.80
1	AA	792	A	C4-C5-N7	-6.15	107.63	110.70
22	BA	1572	A	C4-C5-C6	6.15	120.07	117.00
22	BA	1877	A	C4-C5-C6	6.15	120.08	117.00
22	BA	2761	A	C5-C6-N1	6.15	120.77	117.70
22	BA	149	A	N3-C4-N9	6.15	132.32	127.40
22	BA	2513	A	C5-N7-C8	6.15	106.97	103.90
22	BA	2542	A	N3-C4-N9	6.15	132.32	127.40
1	AA	243	A	C8-N9-C4	6.14	108.26	105.80
1	AA	919	A	C8-N9-C4	6.14	108.26	105.80
1	AA	1176	A	N3-C4-N9	6.14	132.32	127.40
22	BA	661	A	C4-C5-C6	6.14	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	649	A	C8-N9-C4	6.14	108.26	105.80
22	BA	608	A	C4-C5-C6	6.14	120.07	117.00
22	BA	802	A	N3-C4-N9	6.14	132.31	127.40
22	BA	1237	A	N9-C4-C5	6.14	108.26	105.80
1	AA	533	A	C4-C5-N7	-6.14	107.63	110.70
22	BA	1354	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1912	A	C4-C5-C6	6.14	120.07	117.00
1	AA	181	A	C8-N9-C4	6.14	108.25	105.80
22	BA	1050	A	N9-C4-C5	6.14	108.25	105.80
22	BA	1509	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1977	A	C4-C5-C6	6.14	120.07	117.00
22	BA	2037	A	C4-C5-C6	6.14	120.07	117.00
22	BA	761	A	C5-N7-C8	6.13	106.97	103.90
22	BA	1264	A	C8-N9-C4	6.13	108.25	105.80
22	BA	1477	A	N3-C4-N9	6.13	132.31	127.40
22	BA	1876	A	N9-C4-C5	6.13	108.25	105.80
1	AA	129	A	C8-N9-C4	6.13	108.25	105.80
22	BA	2090	A	C4-C5-C6	6.13	120.07	117.00
22	BA	2071	A	C5-C6-N1	6.13	120.77	117.70
22	BA	2031	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1275	A	N3-C4-N9	6.13	132.30	127.40
22	BA	2761	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1146	A	C4-C5-C6	6.13	120.06	117.00
22	BA	925	A	C4-C5-C6	6.13	120.06	117.00
22	BA	2003	A	C4-C5-C6	6.13	120.06	117.00
22	BA	947	A	C8-N9-C4	6.12	108.25	105.80
22	BA	1383	A	C4-C5-C6	6.12	120.06	117.00
1	AA	71	A	C4-C5-N7	-6.12	107.64	110.70
1	AA	749	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1717	A	C5-C6-N1	6.12	120.76	117.70
22	BA	1735	A	C5-C6-N1	6.12	120.76	117.70
1	AA	935	A	C5-C6-N1	6.12	120.76	117.70
22	BA	1014	A	N9-C4-C5	6.12	108.25	105.80
22	BA	1453	A	C8-N9-C4	6.12	108.25	105.80
22	BA	2284	A	C5-C6-N1	6.12	120.76	117.70
1	AA	196	A	C4-C5-C6	6.12	120.06	117.00
1	AA	460	A	C4-C5-C6	6.12	120.06	117.00
22	BA	13	A	N9-C4-C5	6.12	108.25	105.80
22	BA	347	A	C5-C6-N1	6.12	120.76	117.70
22	BA	896	A	N3-C4-N9	6.12	132.30	127.40
22	BA	501	A	C8-N9-C4	6.12	108.25	105.80
22	BA	1142	A	N9-C4-C5	6.12	108.25	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2412	A	N3-C4-N9	6.12	132.30	127.40
1	AA	1188	A	N3-C4-N9	6.12	132.29	127.40
22	BA	631	A	N3-C4-N9	6.12	132.29	127.40
22	BA	735	A	N3-C4-N9	6.12	132.29	127.40
22	BA	1952	A	N3-C4-N9	6.12	132.29	127.40
22	BA	330	A	C5-C6-N1	6.11	120.76	117.70
22	BA	845	A	C4-C5-C6	6.11	120.06	117.00
22	BA	1095	A	C4-C5-N7	-6.11	107.64	110.70
1	AA	270	A	C4-C5-C6	6.11	120.06	117.00
1	AA	675	A	C5-C6-N1	6.11	120.76	117.70
22	BA	556	A	N3-C4-N9	6.11	132.29	127.40
22	BA	807	U	N1-C2-N3	6.11	118.57	114.90
22	BA	933	A	N9-C4-C5	6.11	108.24	105.80
22	BA	1366	A	C8-N9-C4	6.11	108.24	105.80
22	BA	1786	A	C4-C5-C6	6.11	120.06	117.00
22	BA	2282	G	O4'-C1'-N9	6.11	113.09	108.20
23	BB	34	A	C4-C5-N7	-6.11	107.64	110.70
22	BA	207	A	N9-C4-C5	6.11	108.24	105.80
22	BA	1791	A	N3-C4-N9	6.11	132.29	127.40
1	AA	74	A	N9-C4-C5	6.11	108.24	105.80
22	BA	2173	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	2270	A	N3-C4-N9	6.11	132.29	127.40
22	BA	2314	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	2435	A	N3-C4-N9	6.11	132.29	127.40
1	AA	66	A	N3-C4-N9	6.11	132.28	127.40
22	BA	1916	A	N9-C4-C5	6.11	108.24	105.80
22	BA	2765	A	C4-C5-C6	6.11	120.05	117.00
1	AA	554	A	C8-N9-C4	6.10	108.24	105.80
1	AA	1236	A	C5-C6-N1	6.10	120.75	117.70
1	AA	1495	U	C2-N1-C1'	6.10	125.02	117.70
22	BA	340	A	N3-C4-N9	6.10	132.28	127.40
22	BA	706	A	N3-C4-N9	6.10	132.28	127.40
22	BA	979	A	C5-C6-N1	6.10	120.75	117.70
22	BA	1505	A	C8-N9-C4	6.10	108.24	105.80
22	BA	1782	U	O5'-P-OP1	6.10	118.02	110.70
23	BB	73	A	C5-N7-C8	6.10	106.95	103.90
1	AA	149	A	C4-C5-C6	6.10	120.05	117.00
1	AA	704	A	C8-N9-C4	6.10	108.24	105.80
1	AA	1197	A	C4-C5-C6	6.10	120.05	117.00
22	BA	661	A	C8-N9-C4	6.10	108.24	105.80
22	BA	1070	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1067	A	N3-C4-N9	6.10	132.28	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	73	A	C4-C5-C6	6.10	120.05	117.00
22	BA	2009	A	C5-N7-C8	6.10	106.95	103.90
1	AA	602	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1254	A	C8-N9-C4	6.10	108.24	105.80
22	BA	1085	A	C4-C5-C6	6.10	120.05	117.00
22	BA	2705	A	C5-N7-C8	6.10	106.95	103.90
22	BA	1327	A	C5-N7-C8	6.10	106.95	103.90
1	AA	600	A	C8-N9-C4	6.09	108.24	105.80
1	AA	860	A	C4-C5-N7	-6.09	107.65	110.70
22	BA	299	A	C5-C6-N1	6.09	120.75	117.70
22	BA	792	A	C8-N9-C4	6.09	108.24	105.80
22	BA	1679	A	N3-C4-N9	6.09	132.28	127.40
22	BA	1889	A	C4-C5-C6	6.09	120.05	117.00
22	BA	2675	A	C4-C5-C6	6.09	120.05	117.00
55	B8	51	A	C4-C5-C6	6.09	120.05	117.00
55	B8	66	A	N3-C4-N9	6.09	132.28	127.40
1	AA	3	A	N3-C4-N9	6.09	132.27	127.40
1	AA	364	A	C4-C5-N7	-6.09	107.65	110.70
1	AA	1004	A	C4-C5-N7	-6.09	107.65	110.70
1	AA	1368	A	C4-C5-C6	6.09	120.05	117.00
1	AA	1375	A	C8-N9-C4	6.09	108.24	105.80
22	BA	172	A	C8-N9-C4	6.09	108.24	105.80
22	BA	265	A	N3-C4-N9	6.09	132.27	127.40
22	BA	734	A	N3-C4-N9	6.09	132.27	127.40
22	BA	829	A	N3-C4-N9	6.09	132.27	127.40
1	AA	892	A	C4-C5-C6	6.09	120.04	117.00
1	AA	695	A	C8-N9-C4	6.09	108.23	105.80
1	AA	1158	C	N1-C2-O2	6.09	122.55	118.90
22	BA	928	A	C4-C5-C6	6.09	120.04	117.00
55	B8	42	A	N9-C4-C5	6.09	108.23	105.80
22	BA	936	A	C8-N9-C4	6.08	108.23	105.80
22	BA	1205	A	C8-N9-C4	6.08	108.23	105.80
22	BA	2809	A	N3-C4-N9	6.08	132.27	127.40
1	AA	236	A	C8-N9-C4	6.08	108.23	105.80
1	AA	635	A	C8-N9-C4	6.08	108.23	105.80
22	BA	2418	A	N3-C4-N9	6.08	132.26	127.40
22	BA	2425	A	N9-C4-C5	6.08	108.23	105.80
22	BA	1544	A	N9-C4-C5	6.08	108.23	105.80
23	BB	78	A	C8-N9-C4	6.08	108.23	105.80
1	AA	74	A	C8-N9-C4	6.08	108.23	105.80
1	AA	223	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1246	A	C4-C5-N7	-6.08	107.66	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1265	A	N3-C4-N9	6.08	132.26	127.40
1	AA	1157	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	526	A	N9-C4-C5	6.08	108.23	105.80
22	BA	2225	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1900	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1307	A	C4-C5-C6	6.07	120.04	117.00
22	BA	1433	A	C4-C5-C6	6.07	120.04	117.00
22	BA	654	A	C4-C5-C6	6.07	120.04	117.00
22	BA	1544	A	N3-C4-N9	6.07	132.26	127.40
1	AA	246	A	C4-C5-N7	-6.07	107.67	110.70
22	BA	176	A	C4-C5-C6	6.07	120.03	117.00
23	BB	46	A	N3-C4-N9	6.07	132.26	127.40
1	AA	768	A	C8-N9-C4	6.07	108.23	105.80
1	AA	1274	A	C4-C5-C6	6.07	120.03	117.00
22	BA	844	A	C5-C6-N1	6.07	120.73	117.70
22	BA	2542	A	C8-N9-C4	6.07	108.23	105.80
1	AA	139	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1055	A	N3-C4-N9	6.07	132.25	127.40
22	BA	52	A	C8-N9-C4	6.07	108.23	105.80
22	BA	1385	A	C4-C5-N7	-6.07	107.67	110.70
22	BA	2327	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2749	A	N9-C4-C5	6.06	108.22	105.80
1	AA	596	A	C8-N9-C4	6.06	108.22	105.80
22	BA	563	A	C4-C5-N7	-6.06	107.67	110.70
22	BA	2600	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2765	A	C8-N9-C4	6.06	108.22	105.80
22	BA	1871	A	C4-C5-C6	6.06	120.03	117.00
1	AA	349	A	C4-C5-N7	-6.06	107.67	110.70
1	AA	819	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1102	A	C5-C6-N1	6.06	120.73	117.70
22	BA	332	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1085	A	C8-N9-C4	6.06	108.22	105.80
22	BA	1393	A	C8-N9-C4	6.06	108.22	105.80
1	AA	181	A	N3-C4-N9	6.06	132.25	127.40
1	AA	236	A	N3-C4-N9	6.06	132.25	127.40
1	AA	602	A	C8-N9-C4	6.06	108.22	105.80
22	BA	478	A	N3-C4-N9	6.06	132.25	127.40
22	BA	925	A	N3-C4-N9	6.06	132.25	127.40
22	BA	1165	A	N9-C4-C5	6.06	108.22	105.80
22	BA	2725	A	C5-N7-C8	6.06	106.93	103.90
1	AA	621	A	C5-C6-N1	6.06	120.73	117.70
22	BA	241	A	C5-C6-N1	6.06	120.73	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1632	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2171	A	C4-C5-C6	6.05	120.03	117.00
1	AA	767	A	N3-C4-N9	6.05	132.24	127.40
1	AA	1014	A	N3-C4-N9	6.05	132.24	127.40
1	AA	1374	A	C4-C5-C6	6.05	120.03	117.00
22	BA	715	A	C8-N9-C4	6.05	108.22	105.80
22	BA	2031	A	C8-N9-C4	6.05	108.22	105.80
1	AA	496	A	N3-C4-N9	6.05	132.24	127.40
1	AA	807	A	C4-C5-C6	6.05	120.03	117.00
22	BA	1505	A	C4-C5-C6	6.05	120.03	117.00
22	BA	2094	A	C5-C6-N1	6.05	120.72	117.70
22	BA	2886	A	C4-C5-C6	6.05	120.03	117.00
1	AA	729	A	C4-C5-N7	-6.05	107.68	110.70
22	BA	2241	A	C4-C5-C6	6.05	120.02	117.00
1	AA	1191	A	C8-N9-C4	6.05	108.22	105.80
1	AA	1252	A	C4-C5-C6	6.05	120.02	117.00
22	BA	502	A	C4-C5-N7	-6.05	107.68	110.70
22	BA	1469	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1960	A	N3-C4-N9	6.05	132.24	127.40
22	BA	2392	A	C4-C5-C6	6.05	120.02	117.00
22	BA	2241	A	N3-C4-N9	6.04	132.24	127.40
22	BA	2900	A	C4-C5-C6	6.04	120.02	117.00
22	BA	203	A	C5-N7-C8	6.04	106.92	103.90
22	BA	1084	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1307	A	N3-C4-N9	6.04	132.23	127.40
22	BA	1494	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2274	A	C5-N7-C8	6.04	106.92	103.90
22	BA	2516	A	C5-N7-C8	6.04	106.92	103.90
22	BA	352	A	N3-C4-N9	6.04	132.23	127.40
22	BA	1505	A	N3-C4-N9	6.04	132.23	127.40
22	BA	2654	A	N3-C4-N9	6.04	132.23	127.40
23	BB	108	A	N3-C4-N9	6.04	132.23	127.40
1	AA	189	A	C4-C5-C6	6.04	120.02	117.00
1	AA	498	A	C8-N9-C4	6.04	108.22	105.80
1	AA	1150	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1333	A	N9-C4-C5	6.04	108.22	105.80
1	AA	1456	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1260	A	N3-C4-N9	6.04	132.23	127.40
22	BA	1525	A	C5-C6-N1	6.04	120.72	117.70
22	BA	2273	A	C8-N9-C4	6.04	108.22	105.80
22	BA	2434	A	C8-N9-C4	6.04	108.22	105.80
22	BA	2882	A	C8-N9-C4	6.04	108.22	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	155	A	N3-C4-N9	6.04	132.23	127.40
1	AA	873	A	C8-N9-C4	6.04	108.22	105.80
1	AA	1019	A	N3-C4-N9	6.04	132.23	127.40
1	AA	65	A	C8-N9-C4	6.04	108.22	105.80
1	AA	1256	A	N3-C4-N9	6.04	132.23	127.40
22	BA	197	A	N3-C4-N9	6.04	132.23	127.40
22	BA	643	A	C8-N9-C4	6.04	108.21	105.80
22	BA	1244	A	N3-C4-N9	6.04	132.23	127.40
22	BA	1570	A	C5-C6-N1	6.04	120.72	117.70
22	BA	2268	A	C8-N9-C4	6.04	108.21	105.80
22	BA	2392	A	C5-N7-C8	6.04	106.92	103.90
22	BA	1096	A	N3-C4-N9	6.03	132.23	127.40
22	BA	2453	A	N3-C4-N9	6.03	132.23	127.40
22	BA	2814	A	N9-C4-C5	6.03	108.21	105.80
22	BA	2061	G	N3-C4-N9	6.03	129.62	126.00
1	AA	338	A	C5-C6-N1	6.03	120.72	117.70
1	AA	451	A	N3-C4-N9	6.03	132.22	127.40
1	AA	1318	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1534	A	N3-C4-N9	6.03	132.22	127.40
22	BA	482	A	C8-N9-C4	6.03	108.21	105.80
22	BA	928	A	N3-C4-N9	6.03	132.22	127.40
23	BB	39	A	N3-C4-N9	6.03	132.22	127.40
55	B8	41	A	C4-C5-C6	6.03	120.02	117.00
1	AA	325	A	N9-C4-C5	6.03	108.21	105.80
1	AA	1167	A	C5-C6-N1	6.03	120.71	117.70
22	BA	1057	A	C4-C5-C6	6.03	120.01	117.00
22	BA	1142	A	C4-C5-N7	-6.03	107.69	110.70
1	AA	309	A	C4-C5-C6	6.03	120.01	117.00
1	AA	408	A	N3-C4-N9	6.03	132.22	127.40
22	BA	165	A	C4-C5-C6	6.03	120.01	117.00
22	BA	223	A	C4-C5-C6	6.03	120.01	117.00
22	BA	497	A	C5-C6-N1	6.03	120.71	117.70
22	BA	1214	A	C4-C5-C6	6.03	120.01	117.00
22	BA	1244	A	C8-N9-C4	6.03	108.21	105.80
22	BA	1749	A	C8-N9-C4	6.03	108.21	105.80
22	BA	2154	A	C8-N9-C4	6.03	108.21	105.80
23	BB	94	A	C4-C5-N7	-6.03	107.69	110.70
22	BA	602	A	N3-C4-N9	6.02	132.22	127.40
1	AA	3	A	N9-C4-C5	6.02	108.21	105.80
1	AA	119	A	C4-C5-C6	6.02	120.01	117.00
22	BA	1272	A	C4-C5-C6	6.02	120.01	117.00
22	BA	2266	A	N3-C4-N9	6.02	132.22	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	629	A	N3-C4-N9	6.02	132.22	127.40
1	AA	790	A	C8-N9-C4	6.02	108.21	105.80
1	AA	1311	A	N3-C4-N9	6.02	132.22	127.40
22	BA	1353	A	C5-C6-N1	6.02	120.71	117.70
22	BA	1966	A	N9-C4-C5	6.02	108.21	105.80
22	BA	2848	G	O4'-C1'-N9	6.02	113.02	108.20
1	AA	640	A	C8-N9-C4	6.02	108.21	105.80
22	BA	1204	A	C8-N9-C4	6.02	108.21	105.80
22	BA	1890	A	C5-C6-N1	6.02	120.71	117.70
22	BA	2020	A	C4-C5-C6	6.02	120.01	117.00
1	AA	320	A	C5-C6-N1	6.02	120.71	117.70
22	BA	2377	A	C8-N9-C4	6.02	108.21	105.80
22	BA	103	A	C4-C5-C6	6.01	120.01	117.00
22	BA	149	A	C5-N7-C8	6.01	106.91	103.90
22	BA	270	A	N3-C4-N9	6.01	132.21	127.40
22	BA	1095	A	N3-C4-N9	6.01	132.21	127.40
22	BA	2534	A	N9-C4-C5	6.01	108.20	105.80
22	BA	2670	A	N3-C4-N9	6.01	132.21	127.40
22	BA	103	A	N3-C4-N9	6.01	132.21	127.40
22	BA	1433	A	N3-C4-N9	6.01	132.21	127.40
1	AA	913	A	N3-C4-N9	6.01	132.21	127.40
22	BA	144	A	C5-C6-N1	6.01	120.70	117.70
22	BA	675	A	C5-N7-C8	6.01	106.91	103.90
22	BA	1654	A	C8-N9-C4	6.01	108.20	105.80
22	BA	2171	A	C8-N9-C4	6.01	108.20	105.80
22	BA	1553	A	N3-C4-N9	6.01	132.21	127.40
22	BA	2450	A	C5-C6-N1	6.01	120.70	117.70
22	BA	2856	A	C8-N9-C4	6.01	108.20	105.80
1	AA	102	G	N3-C2-N2	6.01	124.11	119.90
1	AA	977	A	C5-C6-N1	6.01	120.70	117.70
22	BA	582	A	C5-N7-C8	6.01	106.90	103.90
22	BA	972	A	N3-C4-N9	6.01	132.21	127.40
22	BA	1597	A	N9-C4-C5	6.00	108.20	105.80
1	AA	1362	A	C5-C6-N1	6.00	120.70	117.70
22	BA	1794	A	N9-C4-C5	6.00	108.20	105.80
1	AA	465	A	C5-C6-N1	6.00	120.70	117.70
1	AA	1319	A	N9-C4-C5	6.00	108.20	105.80
1	AA	1499	A	C4-C5-C6	6.00	120.00	117.00
22	BA	1746	A	N3-C4-N9	6.00	132.20	127.40
22	BA	2169	A	C4-C5-N7	-6.00	107.70	110.70
1	AA	1227	A	N9-C4-C5	6.00	108.20	105.80
22	BA	1342	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1877	A	N3-C4-N9	6.00	132.20	127.40
22	BA	2469	A	N3-C4-N9	6.00	132.20	127.40
1	AA	189	A	N9-C4-C5	6.00	108.20	105.80
1	AA	1288	A	C4-C5-C6	6.00	120.00	117.00
22	BA	190	A	C5-N7-C8	6.00	106.90	103.90
22	BA	196	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	1028	A	N3-C4-N9	6.00	132.20	127.40
1	AA	630	A	C4-C5-C6	6.00	120.00	117.00
1	AA	825	A	N3-C4-N9	5.99	132.19	127.40
1	AA	1434	A	N3-C4-N9	5.99	132.19	127.40
22	BA	1503	A	C4-C5-N7	-5.99	107.70	110.70
1	AA	1508	A	N3-C4-N9	5.99	132.19	127.40
22	BA	654	A	C5-C6-N1	5.99	120.70	117.70
22	BA	1733	G	N1-C6-O6	-5.99	116.31	119.90
22	BA	2311	A	C4-C5-C6	5.99	120.00	117.00
22	BA	1230	A	C4-C5-C6	5.99	120.00	117.00
22	BA	2094	A	N3-C4-N9	5.99	132.19	127.40
22	BA	2154	A	C5-C6-N1	5.99	120.70	117.70
1	AA	1456	A	N3-C4-N9	5.99	132.19	127.40
22	BA	74	A	N3-C4-N9	5.99	132.19	127.40
22	BA	272	A	C5-C6-N1	5.99	120.69	117.70
22	BA	613	A	C8-N9-C4	5.99	108.19	105.80
1	AA	1363	A	N9-C4-C5	5.99	108.19	105.80
22	BA	1549	A	C5-C6-N1	5.99	120.69	117.70
1	AA	595	A	N3-C4-N9	5.99	132.19	127.40
1	AA	807	A	N9-C4-C5	5.99	108.19	105.80
1	AA	1413	A	N3-C4-N9	5.99	132.19	127.40
22	BA	118	A	C8-N9-C4	5.99	108.19	105.80
22	BA	1313	U	C2-N1-C1'	5.99	124.88	117.70
22	BA	2333	A	C4-C5-C6	5.99	119.99	117.00
1	AA	131	A	C8-N9-C4	5.98	108.19	105.80
1	AA	1280	A	C4-C5-C6	5.98	119.99	117.00
22	BA	2154	A	N9-C4-C5	5.98	108.19	105.80
1	AA	195	A	N3-C4-N9	5.98	132.19	127.40
1	AA	777	A	N9-C4-C5	5.98	108.19	105.80
1	AA	1318	A	N3-C4-N9	5.98	132.19	127.40
1	AA	1434	A	C8-N9-C4	5.98	108.19	105.80
22	BA	1347	A	N3-C4-N9	5.98	132.19	127.40
1	AA	223	A	N3-C4-N9	5.98	132.19	127.40
22	BA	1713	A	N9-C4-C5	5.98	108.19	105.80
22	BA	2407	A	C5-C6-N1	5.98	120.69	117.70
1	AA	465	A	C4-C5-C6	5.98	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	546	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1377	A	C4-C5-C6	5.98	119.99	117.00
22	BA	125	A	N3-C4-N9	5.98	132.18	127.40
22	BA	311	A	N9-C4-C5	5.98	108.19	105.80
22	BA	368	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1403	A	C5-C6-N1	5.98	120.69	117.70
22	BA	2037	A	C8-N9-C4	5.98	108.19	105.80
1	AA	65	A	N3-C4-N9	5.98	132.18	127.40
1	AA	1254	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1346	A	C4-C5-C6	5.98	119.99	117.00
22	BA	44	A	N3-C4-N9	5.98	132.18	127.40
22	BA	526	A	C8-N9-C4	5.98	108.19	105.80
22	BA	1978	A	C8-N9-C4	5.98	108.19	105.80
23	BB	104	A	N3-C4-N9	5.98	132.18	127.40
1	AA	706	A	C5-C6-N1	5.98	120.69	117.70
1	AA	174	A	C4-C5-N7	-5.97	107.71	110.70
1	AA	1055	A	C8-N9-C4	5.97	108.19	105.80
1	AA	1311	A	N9-C4-C5	5.97	108.19	105.80
22	BA	142	A	C4-C5-C6	5.97	119.99	117.00
22	BA	984	A	O4'-C1'-N9	5.97	112.98	108.20
22	BA	2033	A	C4-C5-N7	-5.97	107.71	110.70
22	BA	2054	A	C4-C5-N7	-5.97	107.71	110.70
22	BA	2665	A	C5-C6-N1	5.97	120.69	117.70
23	BB	45	A	N9-C4-C5	5.97	108.19	105.80
1	AA	19	A	N3-C4-N9	5.97	132.18	127.40
1	AA	459	A	C4-C5-C6	5.97	119.99	117.00
22	BA	38	A	N3-C4-N9	5.97	132.18	127.40
22	BA	156	A	C5-C6-N1	5.97	120.69	117.70
22	BA	1230	A	N3-C4-N9	5.97	132.18	127.40
22	BA	1321	A	C4-C5-N7	-5.97	107.71	110.70
22	BA	1754	A	N3-C4-N9	5.97	132.18	127.40
1	AA	383	A	C8-N9-C4	5.97	108.19	105.80
22	BA	275	C	C6-N1-C1'	5.97	127.97	120.80
22	BA	478	A	C4-C5-C6	5.97	119.98	117.00
22	BA	917	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2297	A	C4-C5-C6	5.97	119.98	117.00
22	BA	2378	A	C4-C5-C6	5.97	119.98	117.00
22	BA	984	A	C4-C5-C6	5.97	119.98	117.00
22	BA	2322	A	N3-C4-N9	5.97	132.18	127.40
1	AA	1340	A	C5-C6-N1	5.96	120.68	117.70
22	BA	1733	G	C5-C6-O6	5.96	132.18	128.60
1	AA	1110	A	C8-N9-C4	5.96	108.19	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	99	C	N1-C1'-C2'	-5.96	105.44	112.00
1	AA	649	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1446	A	C4-C5-N7	-5.96	107.72	110.70
1	AA	81	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1216	A	C8-N9-C4	5.96	108.18	105.80
22	BA	241	A	N3-C4-N9	5.96	132.17	127.40
22	BA	352	A	C4-C5-C6	5.96	119.98	117.00
22	BA	1244	A	C4-C5-C6	5.96	119.98	117.00
22	BA	1367	A	N3-C4-N9	5.96	132.17	127.40
22	BA	2700	A	C5-C6-N1	5.96	120.68	117.70
22	BA	2705	A	N3-C4-N9	5.96	132.17	127.40
1	AA	784	A	C8-N9-C4	5.96	108.18	105.80
1	AA	1042	A	C4-C5-N7	-5.96	107.72	110.70
22	BA	173	A	C5-C6-N1	5.96	120.68	117.70
22	BA	1127	A	C4-C5-C6	5.96	119.98	117.00
22	BA	1477	A	C8-N9-C4	5.96	108.18	105.80
22	BA	1665	A	C4-C5-N7	-5.96	107.72	110.70
22	BA	1711	A	N3-C4-N9	5.96	132.17	127.40
1	AA	205	A	C8-N9-C4	5.95	108.18	105.80
1	AA	1169	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1180	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1340	A	N3-C4-N9	5.95	132.16	127.40
22	BA	218	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2564	A	N3-C4-N9	5.95	132.16	127.40
1	AA	327	A	N3-C4-N9	5.95	132.16	127.40
1	AA	648	A	C8-N9-C4	5.95	108.18	105.80
1	AA	1014	A	C8-N9-C4	5.95	108.18	105.80
22	BA	226	A	N9-C4-C5	5.95	108.18	105.80
22	BA	715	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2336	A	C8-N9-C4	5.95	108.18	105.80
22	BA	2781	A	C4-C5-C6	5.95	119.97	117.00
1	AA	411	A	N3-C4-N9	5.95	132.16	127.40
22	BA	95	A	N3-C4-N9	5.95	132.16	127.40
22	BA	529	A	C4-C5-C6	5.95	119.97	117.00
22	BA	794	A	C8-N9-C4	5.95	108.18	105.80
22	BA	1614	A	C4-C5-C6	5.95	119.97	117.00
22	BA	177	G	O4'-C1'-N9	5.95	112.96	108.20
22	BA	2670	A	C4-C5-C6	5.95	119.97	117.00
22	BA	727	A	C5-N7-C8	5.95	106.87	103.90
22	BA	1545	A	C8-N9-C4	5.95	108.18	105.80
22	BA	2322	A	C4-C5-C6	5.95	119.97	117.00
22	BA	2572	A	C4-C5-N7	-5.95	107.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1808	A	C4-C5-C6	5.94	119.97	117.00
22	BA	2054	A	N3-C4-N9	5.94	132.16	127.40
1	AA	533	A	C8-N9-C4	5.94	108.18	105.80
1	AA	635	A	N3-C4-N9	5.94	132.15	127.40
1	AA	1349	A	C8-N9-C4	5.94	108.18	105.80
22	BA	631	A	C5-C6-N1	5.94	120.67	117.70
1	AA	325	A	N3-C4-N9	5.94	132.15	127.40
1	AA	520	A	C8-N9-C4	5.94	108.18	105.80
22	BA	10	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1668	A	C5-C6-N1	5.94	120.67	117.70
22	BA	2014	A	N3-C4-N9	5.94	132.15	127.40
22	BA	2154	A	C4-C5-C6	5.94	119.97	117.00
22	BA	2070	A	C5-C6-N1	5.94	120.67	117.70
22	BA	2590	A	C8-N9-C4	5.94	108.18	105.80
1	AA	704	A	C5-C6-N1	5.94	120.67	117.70
22	BA	191	A	C8-N9-C4	5.94	108.17	105.80
22	BA	402	A	N9-C4-C5	5.94	108.17	105.80
22	BA	764	A	N3-C4-N9	5.94	132.15	127.40
23	BB	104	A	C4-C5-C6	5.94	119.97	117.00
1	AA	408	A	C4-C5-N7	-5.94	107.73	110.70
22	BA	457	A	N3-C4-N9	5.94	132.15	127.40
22	BA	936	A	C5-C6-N1	5.94	120.67	117.70
22	BA	1569	A	N3-C4-N9	5.94	132.15	127.40
22	BA	2886	A	N3-C4-N9	5.94	132.15	127.40
1	AA	28	A	C8-N9-C4	5.93	108.17	105.80
1	AA	975	A	C8-N9-C4	5.93	108.17	105.80
22	BA	49	A	C8-N9-C4	5.93	108.17	105.80
22	BA	1111	A	C5-C6-N1	5.93	120.67	117.70
22	BA	1664	A	C4-C5-C6	5.93	119.97	117.00
22	BA	2169	A	N3-C4-N9	5.93	132.15	127.40
22	BA	2632	A	C5-C6-N1	5.93	120.67	117.70
22	BA	2700	A	N3-C4-N9	5.93	132.15	127.40
1	AA	608	A	C5-C6-N1	5.93	120.67	117.70
1	AA	635	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1246	A	C5-C6-N1	5.93	120.67	117.70
1	AA	1410	A	C5-C6-N1	5.93	120.67	117.70
22	BA	10	A	N3-C4-N9	5.93	132.15	127.40
22	BA	1701	A	N9-C4-C5	5.93	108.17	105.80
22	BA	2163	A	C4-C5-N7	-5.93	107.73	110.70
23	BB	50	A	C4-C5-C6	5.93	119.97	117.00
54	B7	9	A	OP1-P-O3'	5.93	118.25	105.20
1	AA	1447	A	C4-C5-C6	5.93	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1650	A	C8-N9-C4	5.93	108.17	105.80
22	BA	2135	A	N3-C4-N9	5.93	132.14	127.40
1	AA	908	A	C8-N9-C4	5.93	108.17	105.80
1	AA	913	A	C8-N9-C4	5.93	108.17	105.80
1	AA	1377	A	C4-C5-N7	-5.93	107.73	110.70
22	BA	1165	A	C4-C5-N7	-5.93	107.73	110.70
22	BA	1755	A	C4-C5-C6	5.93	119.96	117.00
22	BA	2560	A	C5-C6-N1	5.93	120.67	117.70
23	BB	15	A	C5-C6-N1	5.93	120.66	117.70
1	AA	642	A	C8-N9-C4	5.93	108.17	105.80
22	BA	699	A	C8-N9-C4	5.93	108.17	105.80
22	BA	1040	A	C4-C5-C6	5.93	119.96	117.00
1	AA	768	A	C4-C5-N7	-5.93	107.74	110.70
1	AA	845	A	C4-C5-N7	-5.93	107.74	110.70
22	BA	502	A	C5-C6-N1	5.93	120.66	117.70
22	BA	1322	A	N3-C4-N9	5.93	132.14	127.40
1	AA	119	A	C4-C5-N7	-5.92	107.74	110.70
22	BA	324	A	C8-N9-C4	5.92	108.17	105.80
22	BA	1626	A	N3-C4-N9	5.92	132.14	127.40
1	AA	129	A	C4-C5-C6	5.92	119.96	117.00
55	B8	26	A	N9-C4-C5	5.92	108.17	105.80
22	BA	13	A	C5-C6-N1	5.92	120.66	117.70
22	BA	439	A	N9-C4-C5	5.92	108.17	105.80
22	BA	677	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1918	A	C4-C5-C6	5.92	119.96	117.00
1	AA	673	A	C5-C6-N1	5.92	120.66	117.70
1	AA	1289	A	C5-C6-N1	5.92	120.66	117.70
1	AA	1476	A	C5-C6-N1	5.92	120.66	117.70
22	BA	404	A	N3-C4-C5	-5.92	122.66	126.80
1	AA	1374	A	N3-C4-N9	5.92	132.13	127.40
22	BA	454	A	N3-C4-N9	5.92	132.13	127.40
22	BA	563	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1143	A	C8-N9-C4	5.92	108.17	105.80
22	BA	1503	A	C5-C6-N1	5.92	120.66	117.70
1	AA	139	A	C5-C6-N1	5.92	120.66	117.70
1	AA	983	A	C8-N9-C4	5.92	108.17	105.80
22	BA	849	A	C5-N7-C8	5.92	106.86	103.90
22	BA	1569	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1746	A	N9-C4-C5	5.92	108.17	105.80
22	BA	1803	A	C4-C5-C6	5.92	119.96	117.00
1	AA	246	A	C8-N9-C4	5.92	108.17	105.80
1	AA	535	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1431	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1598	A	N3-C4-N9	5.92	132.13	127.40
22	BA	981	A	N9-C4-C5	5.91	108.17	105.80
22	BA	2860	A	C4-C5-C6	5.91	119.96	117.00
1	AA	371	A	C4-C5-C6	5.91	119.96	117.00
22	BA	182	A	N9-C4-C5	5.91	108.17	105.80
22	BA	1359	A	C4-C5-N7	-5.91	107.74	110.70
1	AA	935	A	C4-C5-C6	5.91	119.96	117.00
22	BA	42	A	N3-C4-N9	5.91	132.13	127.40
22	BA	920	A	C4-C5-C6	5.91	119.95	117.00
22	BA	1194	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	2062	A	N9-C4-C5	5.91	108.16	105.80
22	BA	2108	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2564	A	C4-C5-C6	5.91	119.96	117.00
22	BA	2654	A	C5-N7-C8	5.91	106.86	103.90
1	AA	784	A	C5-C6-N1	5.91	120.66	117.70
1	AA	1111	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1492	A	N3-C4-N9	5.91	132.13	127.40
22	BA	299	A	N3-C4-N9	5.91	132.13	127.40
22	BA	644	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	2005	A	C4-C5-C6	5.91	119.95	117.00
22	BA	2171	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2309	A	C4-C5-C6	5.91	119.95	117.00
55	B8	41	A	C5-C6-N1	5.91	120.65	117.70
1	AA	478	A	N3-C4-N9	5.91	132.13	127.40
23	BB	59	A	C8-N9-C4	5.91	108.16	105.80
1	AA	831	A	C8-N9-C4	5.91	108.16	105.80
1	AA	865	A	C5-C6-N1	5.91	120.65	117.70
1	AA	892	A	N3-C4-N9	5.91	132.12	127.40
22	BA	693	A	C5-C6-N1	5.91	120.65	117.70
22	BA	1237	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	1722	A	N3-C4-N9	5.91	132.12	127.40
22	BA	1246	A	N9-C4-C5	5.90	108.16	105.80
1	AA	95	C	C6-N1-C2	-5.90	117.94	120.30
1	AA	845	A	C5-C6-N1	5.90	120.65	117.70
1	AA	1036	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	1919	A	C4-C5-C6	5.90	119.95	117.00
22	BA	2088	A	N3-C4-N9	5.90	132.12	127.40
1	AA	600	A	C5-C6-N1	5.90	120.65	117.70
1	AA	1012	A	C5-C6-N1	5.90	120.65	117.70
1	AA	1441	A	N3-C4-N9	5.90	132.12	127.40
22	BA	345	A	C4-C5-N7	-5.90	107.75	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	627	A	C8-N9-C4	5.90	108.16	105.80
22	BA	877	A	N9-C4-C5	5.90	108.16	105.80
22	BA	1711	A	C5-C6-N1	5.90	120.65	117.70
22	BA	2439	A	C4-C5-C6	5.90	119.95	117.00
22	BA	821	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	1366	A	C4-C5-C6	5.90	119.95	117.00
23	BB	75	G	N3-C4-N9	5.90	129.54	126.00
1	AA	389	A	C8-N9-C4	5.90	108.16	105.80
1	AA	1332	A	N3-C4-N9	5.90	132.12	127.40
22	BA	1069	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1393	A	N9-C4-C5	5.90	108.16	105.80
1	AA	7	A	C4-C5-N7	-5.89	107.75	110.70
1	AA	172	A	N3-C4-N9	5.89	132.12	127.40
1	AA	1151	A	C5-C6-N1	5.89	120.65	117.70
1	AA	1434	A	C4-C5-C6	5.89	119.95	117.00
22	BA	294	A	C4-C5-C6	5.89	119.95	117.00
22	BA	294	A	C5-C6-N1	5.89	120.65	117.70
22	BA	804	A	N3-C4-N9	5.89	132.12	127.40
22	BA	1515	A	C5-C6-N1	5.89	120.65	117.70
1	AA	19	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	733	G	C5-N7-C8	-5.89	101.35	104.30
22	BA	1304	A	C4-C5-C6	5.89	119.95	117.00
22	BA	1801	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	1805	A	N3-C4-N9	5.89	132.11	127.40
22	BA	1858	A	C5-C6-N1	5.89	120.65	117.70
22	BA	1912	A	C4-C5-N7	-5.89	107.75	110.70
1	AA	1180	A	C4-C5-C6	5.89	119.94	117.00
22	BA	241	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1918	A	N9-C4-C5	5.89	108.16	105.80
22	BA	2088	A	C4-C5-C6	5.89	119.94	117.00
22	BA	2101	A	N3-C4-N9	5.89	132.11	127.40
1	AA	414	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1299	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1319	A	C8-N9-C4	5.89	108.16	105.80
22	BA	1276	A	C8-N9-C4	5.89	108.16	105.80
1	AA	81	A	N3-C4-N9	5.89	132.11	127.40
1	AA	288	A	N3-C4-N9	5.89	132.11	127.40
1	AA	313	A	N9-C4-C5	5.89	108.15	105.80
1	AA	572	A	C4-C5-C6	5.89	119.94	117.00
22	BA	340	A	C8-N9-C4	5.89	108.16	105.80
1	AA	282	A	N3-C4-N9	5.88	132.11	127.40
1	AA	1349	A	N3-C4-N9	5.88	132.11	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2741	A	N9-C4-C5	5.88	108.15	105.80
22	BA	637	A	C5-C6-N1	5.88	120.64	117.70
22	BA	1496	A	N3-C4-N9	5.88	132.11	127.40
1	AA	77	A	N3-C4-N9	5.88	132.10	127.40
1	AA	336	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	294	A	C8-N9-C4	5.88	108.15	105.80
22	BA	368	A	N3-C4-N9	5.88	132.11	127.40
22	BA	996	A	N3-C4-N9	5.88	132.10	127.40
22	BA	2821	A	C4-C5-C6	5.88	119.94	117.00
1	AA	263	A	C8-N9-C4	5.88	108.15	105.80
1	AA	1349	A	C4-C5-C6	5.88	119.94	117.00
22	BA	477	A	C8-N9-C4	5.88	108.15	105.80
22	BA	1916	A	C4-C5-C6	5.88	119.94	117.00
22	BA	2632	A	C4-C5-N7	-5.88	107.76	110.70
1	AA	1429	A	C5-C6-N1	5.88	120.64	117.70
22	BA	53	A	N9-C4-C5	5.88	108.15	105.80
22	BA	91	A	N3-C4-N9	5.88	132.10	127.40
22	BA	2850	A	C8-N9-C4	5.88	108.15	105.80
22	BA	1020	A	N3-C4-N9	5.88	132.10	127.40
22	BA	1133	A	C5-C6-N1	5.88	120.64	117.70
22	BA	1392	A	C8-N9-C4	5.88	108.15	105.80
22	BA	1744	A	N3-C4-N9	5.88	132.10	127.40
1	AA	432	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1155	A	N3-C4-N9	5.87	132.10	127.40
22	BA	603	A	C4-C5-N7	-5.87	107.76	110.70
22	BA	1749	A	C4-C5-C6	5.87	119.94	117.00
22	BA	1749	A	N9-C4-C5	5.87	108.15	105.80
22	BA	2598	A	C8-N9-C4	5.87	108.15	105.80
22	BA	685	A	N9-C4-C5	5.87	108.15	105.80
22	BA	783	A	C8-N9-C4	5.87	108.15	105.80
22	BA	1927	A	C5-C6-N1	5.87	120.64	117.70
22	BA	1960	A	C8-N9-C4	5.87	108.15	105.80
22	BA	2590	A	N3-C4-N9	5.87	132.10	127.40
23	BB	66	A	C5-N7-C8	5.87	106.84	103.90
22	BA	332	A	C8-N9-C4	5.87	108.15	105.80
1	AA	478	A	N9-C4-C5	5.87	108.15	105.80
1	AA	1437	A	N9-C4-C5	5.87	108.15	105.80
22	BA	173	A	C4-C5-C6	5.87	119.93	117.00
22	BA	1057	A	N9-C4-C5	5.87	108.15	105.80
22	BA	2154	A	N3-C4-N9	5.87	132.09	127.40
22	BA	38	A	C4-C5-C6	5.87	119.93	117.00
22	BA	1085	A	N9-C4-C5	5.87	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	687	A	C4-C5-N7	-5.87	107.77	110.70
22	BA	279	A	N3-C4-N9	5.87	132.09	127.40
22	BA	2887	A	N3-C4-N9	5.87	132.09	127.40
22	BA	453	A	N3-C4-N9	5.86	132.09	127.40
22	BA	2453	A	C5-C6-N1	5.86	120.63	117.70
55	B8	21	A	C8-N9-C4	5.86	108.15	105.80
22	BA	1569	A	C8-N9-C4	5.86	108.14	105.80
22	BA	2887	A	C4-C5-C6	5.86	119.93	117.00
22	BA	74	A	C5-C6-N1	5.86	120.63	117.70
22	BA	1005	C	C6-N1-C2	-5.86	117.95	120.30
22	BA	1548	A	C5-N7-C8	5.86	106.83	103.90
22	BA	2513	A	C4-C5-C6	5.86	119.93	117.00
22	BA	920	A	C5-C6-N1	5.86	120.63	117.70
22	BA	1745	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1531	A	N3-C4-N9	5.86	132.09	127.40
22	BA	310	A	N9-C4-C5	5.86	108.14	105.80
22	BA	1918	A	C8-N9-C4	5.86	108.14	105.80
22	BA	2665	A	C4-C5-C6	5.86	119.93	117.00
1	AA	65	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1042	A	C5-C6-N1	5.86	120.63	117.70
22	BA	443	A	N3-C4-N9	5.86	132.08	127.40
22	BA	716	A	C4-C5-C6	5.86	119.93	117.00
22	BA	1127	A	C8-N9-C4	5.86	108.14	105.80
22	BA	1664	A	N3-C4-N9	5.86	132.09	127.40
1	AA	969	A	C4-C5-C6	5.85	119.93	117.00
22	BA	83	A	C4-C5-C6	5.85	119.93	117.00
22	BA	155	A	C5-C6-N1	5.85	120.63	117.70
1	AA	502	A	C5-C6-N1	5.85	120.63	117.70
1	AA	1360	A	N3-C4-N9	5.85	132.08	127.40
22	BA	182	A	C4-C5-N7	-5.85	107.77	110.70
22	BA	1759	A	C4-C5-C6	5.85	119.93	117.00
1	AA	1157	A	N3-C4-N9	5.85	132.08	127.40
22	BA	44	A	N9-C4-C5	5.85	108.14	105.80
22	BA	1614	A	C8-N9-C4	5.85	108.14	105.80
22	BA	2101	A	C4-C5-N7	-5.85	107.78	110.70
22	BA	2346	A	N3-C4-N9	5.85	132.08	127.40
1	AA	663	A	N3-C4-N9	5.85	132.08	127.40
1	AA	937	A	N3-C4-N9	5.85	132.08	127.40
22	BA	877	A	C8-N9-C4	5.85	108.14	105.80
22	BA	1244	A	N9-C4-C5	5.85	108.14	105.80
1	AA	1413	A	C4-C5-C6	5.85	119.92	117.00
22	BA	118	A	C5-C6-N1	5.85	120.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	300	A	N9-C4-C5	5.85	108.14	105.80
22	BA	1008	A	C4-C5-C6	5.85	119.92	117.00
22	BA	2013	A	C8-N9-C4	5.85	108.14	105.80
1	AA	602	A	C4-C5-C6	5.85	119.92	117.00
1	AA	607	A	C4-C5-C6	5.85	119.92	117.00
22	BA	2721	A	C5-N7-C8	5.85	106.82	103.90
22	BA	2753	A	N9-C4-C5	5.84	108.14	105.80
1	AA	1046	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2879	A	C8-N9-C4	5.84	108.14	105.80
1	AA	389	A	C5-C6-N1	5.84	120.62	117.70
1	AA	1502	A	N3-C4-N9	5.84	132.07	127.40
22	BA	1008	A	N3-C4-N9	5.84	132.07	127.40
22	BA	2270	A	C8-N9-C4	5.84	108.14	105.80
1	AA	1299	A	C8-N9-C4	5.84	108.14	105.80
22	BA	556	A	C4-C5-C6	5.84	119.92	117.00
22	BA	1008	A	N9-C4-C5	5.84	108.14	105.80
22	BA	2814	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1179	A	C5-C6-N1	5.84	120.62	117.70
22	BA	1420	A	N3-C4-N9	5.84	132.07	127.40
22	BA	126	A	C5-C6-N1	5.84	120.62	117.70
22	BA	482	A	C5-N7-C8	5.84	106.82	103.90
22	BA	1596	A	N3-C4-N9	5.84	132.07	127.40
22	BA	2158	A	C4-C5-N7	-5.84	107.78	110.70
22	BA	2199	A	C8-N9-C4	5.84	108.14	105.80
23	BB	104	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2169	A	N9-C4-C5	5.83	108.13	105.80
1	AA	109	A	N3-C4-N9	5.83	132.07	127.40
1	AA	563	A	C5-C6-N1	5.83	120.62	117.70
1	AA	1000	A	N3-C4-N9	5.83	132.07	127.40
1	AA	1246	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	1803	A	C5-N7-C8	5.83	106.82	103.90
1	AA	694	A	C4-C5-C6	5.83	119.92	117.00
22	BA	299	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	1838	C	C6-N1-C2	-5.83	117.97	120.30
22	BA	1927	A	N3-C4-N9	5.83	132.06	127.40
22	BA	2268	A	N3-C4-N9	5.83	132.06	127.40
22	BA	207	A	C8-N9-C4	5.83	108.13	105.80
22	BA	222	A	C5-C6-N1	5.83	120.61	117.70
22	BA	792	A	N3-C4-N9	5.83	132.06	127.40
1	AA	50	A	C8-N9-C4	5.83	108.13	105.80
1	AA	195	A	C8-N9-C4	5.83	108.13	105.80
22	BA	1603	A	N3-C4-N9	5.83	132.06	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2198	A	N3-C4-N9	5.83	132.06	127.40
22	BA	2632	A	N3-C4-N9	5.83	132.06	127.40
1	AA	315	A	C4-C5-N7	-5.83	107.79	110.70
1	AA	749	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1311	A	C5-C6-N1	5.83	120.61	117.70
1	AA	1408	A	N3-C4-N9	5.83	132.06	127.40
22	BA	181	A	C4-C5-C6	5.83	119.91	117.00
22	BA	609	A	C4-C5-C6	5.83	119.91	117.00
22	BA	1504	A	C4-C5-C6	5.83	119.91	117.00
1	AA	28	A	C4-C5-C6	5.82	119.91	117.00
1	AA	69	G	N1-C2-N2	-5.82	110.96	116.20
1	AA	174	A	C5-C6-N1	5.82	120.61	117.70
22	BA	661	A	N9-C4-C5	5.82	108.13	105.80
55	B8	26	A	C5-C6-N1	5.82	120.61	117.70
1	AA	845	A	N3-C4-N9	5.82	132.06	127.40
22	BA	73	A	N9-C4-C5	5.82	108.13	105.80
1	AA	1254	A	N3-C4-N9	5.82	132.06	127.40
22	BA	83	A	C5-C6-N1	5.82	120.61	117.70
22	BA	1365	A	C5-C6-N1	5.82	120.61	117.70
22	BA	1632	A	C5-C6-N1	5.82	120.61	117.70
22	BA	2369	A	C4-C5-C6	5.82	119.91	117.00
22	BA	2873	A	C8-N9-C4	5.82	108.13	105.80
1	AA	344	A	N9-C4-C5	5.82	108.13	105.80
1	AA	602	A	C5-C6-N1	5.82	120.61	117.70
1	AA	1248	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1288	A	N9-C4-C5	5.82	108.13	105.80
22	BA	197	A	C5-N7-C8	5.82	106.81	103.90
22	BA	1637	A	C5-C6-N1	5.82	120.61	117.70
22	BA	2070	A	N3-C4-N9	5.82	132.05	127.40
22	BA	1655	A	N3-C4-N9	5.82	132.05	127.40
22	BA	1717	A	N3-C4-N9	5.82	132.05	127.40
22	BA	1805	A	N9-C4-C5	5.82	108.13	105.80
22	BA	1918	A	C4-C5-N7	-5.82	107.79	110.70
1	AA	179	A	C4-C5-C6	5.81	119.91	117.00
1	AA	1151	A	C4-C5-C6	5.81	119.91	117.00
22	BA	345	A	N9-C4-C5	5.81	108.13	105.80
22	BA	1084	A	C4-C5-N7	-5.81	107.79	110.70
22	BA	2309	A	N3-C4-N9	5.81	132.05	127.40
22	BA	547	A	C4-C5-N7	-5.81	107.79	110.70
22	BA	927	A	C4-C5-C6	5.81	119.91	117.00
22	BA	1787	A	C8-N9-C4	5.81	108.12	105.80
22	BA	2094	A	C4-C5-C6	5.81	119.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2547	A	N9-C4-C5	5.81	108.12	105.80
22	BA	152	A	C5-C6-N1	5.81	120.61	117.70
22	BA	925	A	C5-C6-N1	5.81	120.61	117.70
22	BA	1214	A	N3-C4-N9	5.81	132.05	127.40
1	AA	16	A	C8-N9-C4	5.81	108.12	105.80
1	AA	167	A	C5-C6-N1	5.81	120.61	117.70
1	AA	1036	A	N9-C4-C5	5.81	108.12	105.80
22	BA	602	A	C5-C6-N1	5.81	120.61	117.70
22	BA	756	A	N3-C4-N9	5.81	132.05	127.40
22	BA	1453	A	C4-C5-C6	5.81	119.91	117.00
22	BA	160	A	N3-C4-N9	5.81	132.05	127.40
22	BA	985	C	C6-N1-C2	-5.81	117.98	120.30
22	BA	990	A	C4-C5-C6	5.81	119.90	117.00
22	BA	1262	A	C4-C5-N7	-5.81	107.80	110.70
22	BA	2191	A	N9-C4-C5	5.81	108.12	105.80
22	BA	2212	A	C8-N9-C4	5.81	108.12	105.80
22	BA	483	A	N3-C4-N9	5.81	132.04	127.40
22	BA	666	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	927	A	C5-C6-N1	5.80	120.60	117.70
22	BA	1014	A	C8-N9-C4	5.80	108.12	105.80
22	BA	2426	A	N3-C4-N9	5.80	132.04	127.40
1	AA	607	A	N3-C4-N9	5.80	132.04	127.40
1	AA	595	A	N9-C4-C5	5.80	108.12	105.80
22	BA	609	A	N3-C4-N9	5.80	132.04	127.40
22	BA	633	A	N3-C4-N9	5.80	132.04	127.40
22	BA	1054	A	C5-C6-N1	5.80	120.60	117.70
22	BA	1070	A	C8-N9-C4	5.80	108.12	105.80
22	BA	1676	A	C4-C5-C6	5.80	119.90	117.00
22	BA	2314	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2336	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2821	A	C5-C6-N1	5.80	120.60	117.70
1	AA	50	A	C4-C5-C6	5.80	119.90	117.00
1	AA	81	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1900	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1968	G	C8-N9-C4	5.80	108.72	106.40
22	BA	294	A	N9-C4-C5	5.80	108.12	105.80
22	BA	1327	A	C8-N9-C4	5.80	108.12	105.80
1	AA	792	A	C4-C5-C6	5.80	119.90	117.00
22	BA	125	A	C4-C5-C6	5.80	119.90	117.00
22	BA	1009	A	C4-C5-C6	5.80	119.90	117.00
23	BB	46	A	N9-C4-C5	5.80	108.12	105.80
1	AA	192	A	C4-C5-N7	-5.79	107.80	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	648	A	N9-C4-C5	5.79	108.12	105.80
1	AA	1357	A	N3-C4-N9	5.79	132.04	127.40
22	BA	332	A	C4-C5-N7	-5.79	107.80	110.70
1	AA	1480	A	C4-C5-C6	5.79	119.90	117.00
22	BA	479	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2327	A	N9-C4-C5	5.79	108.12	105.80
22	BA	819	A	C4-C5-C6	5.79	119.90	117.00
22	BA	1027	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2270	A	C5-C6-N1	5.79	120.60	117.70
22	BA	2670	A	C5-C6-N1	5.79	120.60	117.70
1	AA	1333	A	C8-N9-C4	5.79	108.12	105.80
22	BA	374	A	C4-C5-N7	-5.79	107.81	110.70
22	BA	538	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1919	A	C8-N9-C4	5.79	108.12	105.80
1	AA	282	A	C5-C6-N1	5.79	120.59	117.70
1	AA	432	A	C8-N9-C4	5.79	108.11	105.80
22	BA	38	A	C5-C6-N1	5.79	120.59	117.70
22	BA	2101	A	C5-C6-N1	5.79	120.59	117.70
1	AA	1418	A	C8-N9-C4	5.79	108.11	105.80
22	BA	2335	A	N3-C4-N9	5.79	132.03	127.40
1	AA	397	A	C5-C6-N1	5.79	120.59	117.70
1	AA	1176	A	C8-N9-C4	5.79	108.11	105.80
22	BA	94	A	N3-C4-N9	5.79	132.03	127.40
22	BA	739	A	C5-N7-C8	5.79	106.79	103.90
22	BA	959	A	C8-N9-C4	5.79	108.11	105.80
1	AA	309	A	N3-C4-N9	5.78	132.03	127.40
1	AA	1204	A	N9-C4-C5	5.78	108.11	105.80
22	BA	2823	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1229	A	C5-C6-N1	5.78	120.59	117.70
1	AA	1465	A	N3-C4-N9	5.78	132.03	127.40
22	BA	454	A	N9-C4-C5	5.78	108.11	105.80
22	BA	673	C	N1-C2-N3	5.78	123.25	119.20
1	AA	59	A	C4-C5-C6	5.78	119.89	117.00
1	AA	621	A	C4-C5-N7	-5.78	107.81	110.70
1	AA	1350	A	C8-N9-C4	5.78	108.11	105.80
1	AA	996	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1428	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1434	A	C5-C6-N1	5.78	120.59	117.70
1	AA	1204	A	C8-N9-C4	5.78	108.11	105.80
22	BA	182	A	C5-C6-N1	5.78	120.59	117.70
22	BA	2019	A	C5-N7-C8	5.78	106.79	103.90
22	BA	142	A	N9-C4-C5	5.77	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1098	A	C4-C5-N7	-5.77	107.81	110.70
22	BA	1403	A	N3-C4-N9	5.77	132.02	127.40
22	BA	2267	A	C4-C5-C6	5.77	119.89	117.00
1	AA	102	G	N3-C4-C5	-5.77	125.71	128.60
1	AA	782	A	N3-C4-N9	5.77	132.02	127.40
1	AA	1410	A	N3-C4-N9	5.77	132.02	127.40
1	AA	819	A	C4-C5-C6	5.77	119.89	117.00
22	BA	221	A	N3-C4-N9	5.77	132.02	127.40
1	AA	547	A	C8-N9-C4	5.77	108.11	105.80
1	AA	1035	A	C5-C6-N1	5.77	120.58	117.70
22	BA	2725	A	C8-N9-C4	5.77	108.11	105.80
22	BA	2781	A	C5-C6-N1	5.77	120.58	117.70
1	AA	1500	A	C4-C5-C6	5.77	119.88	117.00
22	BA	231	A	N9-C4-C5	5.77	108.11	105.80
22	BA	1286	A	C8-N9-C4	5.77	108.11	105.80
22	BA	1677	A	C8-N9-C4	5.77	108.11	105.80
22	BA	2094	A	C8-N9-C4	5.77	108.11	105.80
22	BA	582	A	N3-C4-N9	5.77	132.01	127.40
22	BA	626	A	C5-N7-C8	5.77	106.78	103.90
55	B8	38	A	C8-N9-C4	5.77	108.11	105.80
22	BA	1966	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	63	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1700	A	N3-C4-N9	5.76	132.01	127.40
1	AA	412	A	N9-C4-C5	5.76	108.10	105.80
22	BA	800	A	N9-C4-C5	5.76	108.10	105.80
22	BA	1080	A	C4-C5-C6	5.76	119.88	117.00
22	BA	1570	A	C5-N7-C8	5.76	106.78	103.90
23	BB	119	A	C4-C5-C6	5.76	119.88	117.00
1	AA	192	A	N3-C4-N9	5.76	132.01	127.40
1	AA	1093	A	N3-C4-N9	5.76	132.01	127.40
1	AA	1333	A	C4-C5-C6	5.76	119.88	117.00
1	AA	1492	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	1591	A	C4-C5-C6	5.76	119.88	117.00
22	BA	1610	A	C8-N9-C4	5.76	108.10	105.80
22	BA	1713	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2205	A	N9-C4-C5	5.76	108.10	105.80
1	AA	1437	A	N3-C4-N9	5.76	132.01	127.40
22	BA	477	A	N3-C4-N9	5.76	132.01	127.40
1	AA	338	A	C8-N9-C4	5.76	108.10	105.80
1	AA	509	A	C8-N9-C4	5.76	108.10	105.80
1	AA	655	A	C5-C6-N1	5.76	120.58	117.70
1	AA	1318	A	C8-N9-C4	5.76	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1410	A	N9-C4-C5	5.76	108.10	105.80
22	BA	52	A	N3-C4-N9	5.76	132.00	127.40
22	BA	792	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	2051	A	N9-C4-C5	5.76	108.10	105.80
22	BA	2497	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	2748	A	C8-N9-C4	5.76	108.10	105.80
55	B8	51	A	N9-C4-C5	5.76	108.10	105.80
1	AA	712	A	C4-C5-C6	5.75	119.88	117.00
22	BA	1308	A	N3-C4-N9	5.75	132.00	127.40
22	BA	2019	A	C5-C6-N1	5.75	120.58	117.70
22	BA	2160	C	N1-C2-O2	5.75	122.35	118.90
23	BB	50	A	N3-C4-N9	5.75	132.00	127.40
22	BA	528	A	C4-C5-C6	5.75	119.88	117.00
22	BA	878	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1717	A	C4-C5-C6	5.75	119.88	117.00
1	AA	195	A	C5-C6-N1	5.75	120.58	117.70
22	BA	1080	A	C4-C5-N7	-5.75	107.82	110.70
22	BA	1095	A	C5-C6-N1	5.75	120.58	117.70
22	BA	1274	A	C8-N9-C4	5.75	108.10	105.80
22	BA	1890	A	N3-C4-N9	5.75	132.00	127.40
22	BA	2267	A	C8-N9-C4	5.75	108.10	105.80
1	AA	435	A	C4-C5-C6	5.75	119.88	117.00
1	AA	665	A	C5-C6-N1	5.75	120.58	117.70
1	AA	747	A	C5-C6-N1	5.75	120.58	117.70
22	BA	412	A	N9-C4-C5	5.75	108.10	105.80
22	BA	505	A	N3-C4-N9	5.75	132.00	127.40
1	AA	253	A	N3-C4-N9	5.75	132.00	127.40
1	AA	716	A	C4-C5-C6	5.75	119.88	117.00
1	AA	718	A	C8-N9-C4	5.75	108.10	105.80
22	BA	415	A	C8-N9-C4	5.75	108.10	105.80
22	BA	1155	A	C5-C6-N1	5.75	120.58	117.70
22	BA	1713	A	C4-C5-N7	-5.75	107.83	110.70
22	BA	2660	A	N9-C4-C5	5.75	108.10	105.80
23	BB	75	G	N3-C4-C5	-5.75	125.73	128.60
55	B8	69	A	C8-N9-C4	5.75	108.10	105.80
1	AA	600	A	N9-C4-C5	5.75	108.10	105.80
1	AA	1204	A	C4-C5-C6	5.75	119.87	117.00
22	BA	666	A	N9-C4-C5	5.75	108.10	105.80
22	BA	1147	A	C8-N9-C4	5.75	108.10	105.80
22	BA	1780	A	N9-C4-C5	5.75	108.10	105.80
22	BA	2052	A	C8-N9-C4	5.75	108.10	105.80
22	BA	2080	A	C4-C5-C6	5.75	119.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	42	A	C4-C5-C6	5.75	119.87	117.00
22	BA	2037	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1377	A	N9-C4-C5	5.74	108.10	105.80
22	BA	861	A	C8-N9-C4	5.74	108.10	105.80
22	BA	1749	A	N3-C4-N9	5.74	132.00	127.40
22	BA	1803	A	N3-C4-N9	5.74	132.00	127.40
22	BA	730	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1783	A	C4-C5-C6	5.74	119.87	117.00
1	AA	69	G	N1-C6-O6	-5.74	116.46	119.90
22	BA	1713	A	C8-N9-C4	5.74	108.09	105.80
1	AA	574	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1021	A	C8-N9-C4	5.74	108.09	105.80
1	AA	1101	A	C5-C6-N1	5.74	120.57	117.70
22	BA	262	A	N3-C4-N9	5.74	131.99	127.40
22	BA	502	A	N3-C4-N9	5.74	131.99	127.40
22	BA	2054	A	C5-C6-N1	5.74	120.57	117.70
1	AA	440	C	N1-C2-O2	5.73	122.34	118.90
1	AA	622	A	C5-C6-N1	5.73	120.57	117.70
8	AH	96	MET	CA-CB-CG	5.73	123.05	113.30
1	AA	1287	A	C8-N9-C4	5.73	108.09	105.80
22	BA	1089	A	N3-C4-N9	5.73	131.99	127.40
22	BA	1366	A	N3-C4-N9	5.73	131.99	127.40
22	BA	1597	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	182	A	C5-C6-N1	5.73	120.56	117.70
22	BA	1932	A	N9-C4-C5	5.73	108.09	105.80
55	B8	73	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	393	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1269	A	C4-C5-C6	5.73	119.86	117.00
22	BA	2297	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	189	A	C4-C5-N7	-5.73	107.84	110.70
1	AA	1092	A	C4-C5-C6	5.73	119.86	117.00
1	AA	1163	A	C5-C6-N1	5.73	120.56	117.70
22	BA	324	A	N3-C4-N9	5.73	131.98	127.40
22	BA	563	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1420	A	C5-C6-N1	5.73	120.56	117.70
22	BA	1998	A	N3-C4-N9	5.73	131.98	127.40
1	AA	371	A	C5-C6-N1	5.73	120.56	117.70
22	BA	382	A	C5-C6-N1	5.73	120.56	117.70
22	BA	905	A	C4-C5-N7	-5.73	107.84	110.70
22	BA	1088	A	C4-C5-C6	5.73	119.86	117.00
22	BA	1155	A	C4-C5-C6	5.73	119.86	117.00
1	AA	2	A	C8-N9-C4	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	222	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	1829	A	N9-C4-C5	5.72	108.09	105.80
1	AA	32	A	C8-N9-C4	5.72	108.09	105.80
1	AA	1368	A	N3-C4-N9	5.72	131.98	127.40
22	BA	6	A	C4-C5-C6	5.72	119.86	117.00
22	BA	941	A	C4-C5-C6	5.72	119.86	117.00
1	AA	687	A	N3-C4-N9	5.72	131.97	127.40
1	AA	1101	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1507	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	142	A	C5-C6-N1	5.72	120.56	117.70
22	BA	1287	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1912	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2706	A	C5-C6-N1	5.72	120.56	117.70
1	AA	1507	A	N3-C4-N9	5.72	131.97	127.40
22	BA	514	A	C5-C6-N1	5.72	120.56	117.70
22	BA	1014	A	C4-C5-C6	5.72	119.86	117.00
22	BA	1788	C	C6-N1-C2	-5.71	118.01	120.30
22	BA	2058	A	C4-C5-C6	5.71	119.86	117.00
22	BA	2511	U	C6-N1-C2	-5.71	117.57	121.00
22	BA	2547	A	C8-N9-C4	5.71	108.09	105.80
1	AA	71	A	C5-C6-N1	5.71	120.56	117.70
1	AA	196	A	C8-N9-C4	5.71	108.08	105.80
1	AA	977	A	C4-C5-C6	5.71	119.86	117.00
22	BA	89	A	N9-C4-C5	5.71	108.08	105.80
22	BA	1532	A	C4-C5-C6	5.71	119.86	117.00
22	BA	2297	A	N9-C4-C5	5.71	108.08	105.80
1	AA	919	A	C4-C5-C6	5.71	119.86	117.00
22	BA	508	A	C5-C6-N1	5.71	120.56	117.70
22	BA	761	A	C5-C6-N1	5.71	120.56	117.70
22	BA	1570	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2534	A	N3-C4-N9	5.71	131.97	127.40
1	AA	263	A	N9-C4-C5	5.71	108.08	105.80
1	AA	303	A	N3-C4-N9	5.71	131.97	127.40
1	AA	495	A	N3-C4-N9	5.71	131.97	127.40
1	AA	546	A	C5-C6-N1	5.71	120.55	117.70
1	AA	969	A	N9-C4-C5	5.71	108.08	105.80
22	BA	941	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2173	A	N3-C4-N9	5.71	131.97	127.40
1	AA	263	A	N3-C4-N9	5.71	131.97	127.40
1	AA	535	A	N3-C4-N9	5.71	131.97	127.40
22	BA	422	A	C5-C6-N1	5.71	120.55	117.70
1	AA	1257	A	N3-C4-N9	5.71	131.96	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2	A	C5-C6-N1	5.70	120.55	117.70
22	BA	1393	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	1551	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	2241	A	C5-C6-N1	5.70	120.55	117.70
22	BA	2333	A	C5-C6-N1	5.70	120.55	117.70
22	BA	2776	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	978	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	2275	C	C6-N1-C2	-5.70	118.02	120.30
1	AA	336	A	C5-C6-N1	5.70	120.55	117.70
1	AA	807	A	C5-C6-N1	5.70	120.55	117.70
1	AA	892	A	C8-N9-C4	5.70	108.08	105.80
22	BA	477	A	C4-C5-C6	5.70	119.85	117.00
22	BA	626	A	N3-C4-N9	5.70	131.96	127.40
22	BA	1504	A	C5-C6-N1	5.70	120.55	117.70
1	AA	263	A	C4-C5-C6	5.70	119.85	117.00
1	AA	595	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	556	A	C8-N9-C4	5.70	108.08	105.80
22	BA	756	A	C5-C6-N1	5.70	120.55	117.70
22	BA	1928	A	N9-C4-C5	5.70	108.08	105.80
22	BA	2427	C	OP1-P-O3'	5.70	117.73	105.20
22	BA	2851	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1410	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	172	A	C5-C6-N1	5.70	120.55	117.70
22	BA	833	A	N3-C4-N9	5.70	131.96	127.40
22	BA	878	A	C4-C5-C6	5.70	119.85	117.00
22	BA	2792	A	C5-C6-N1	5.70	120.55	117.70
1	AA	1333	A	N3-C4-N9	5.69	131.96	127.40
22	BA	1535	A	N3-C4-N9	5.69	131.96	127.40
1	AA	1	A	C8-N9-C4	5.69	108.08	105.80
1	AA	1503	A	N3-C4-N9	5.69	131.95	127.40
22	BA	218	A	C5-N7-C8	5.69	106.75	103.90
22	BA	988	A	N3-C4-N9	5.69	131.96	127.40
22	BA	2764	A	N3-C4-N9	5.69	131.95	127.40
1	AA	743	A	N3-C4-N9	5.69	131.95	127.40
1	AA	749	A	C8-N9-C4	5.69	108.08	105.80
22	BA	404	A	C5-N7-C8	5.69	106.75	103.90
22	BA	1579	A	C5-C6-N1	5.69	120.55	117.70
22	BA	1630	A	C4-C5-C6	5.69	119.84	117.00
22	BA	1759	A	C5-C6-N1	5.69	120.55	117.70
1	AA	2	A	N9-C4-C5	5.69	108.08	105.80
1	AA	1357	A	C4-C5-C6	5.69	119.84	117.00
22	BA	802	A	C4-C5-N7	-5.69	107.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	973	A	C4-C5-C6	5.69	119.84	117.00
1	AA	320	A	N3-C4-N9	5.69	131.95	127.40
1	AA	649	A	N3-C4-N9	5.69	131.95	127.40
22	BA	119	A	C5-C6-N1	5.69	120.54	117.70
22	BA	152	A	N3-C4-N9	5.69	131.95	127.40
22	BA	216	A	N9-C4-C5	5.69	108.08	105.80
22	BA	1098	A	N3-C4-N9	5.69	131.95	127.40
22	BA	1586	A	C4-C5-C6	5.69	119.84	117.00
22	BA	2013	A	N3-C4-N9	5.69	131.95	127.40
22	BA	2899	A	C5-C6-N1	5.69	120.54	117.70
1	AA	26	A	C8-N9-C4	5.69	108.07	105.80
1	AA	1155	A	C4-C5-C6	5.69	119.84	117.00
1	AA	1155	A	C5-C6-N1	5.69	120.54	117.70
22	BA	512	G	N1-C6-O6	-5.68	116.49	119.90
22	BA	2468	A	C5-C6-N1	5.68	120.54	117.70
22	BA	2738	A	N9-C4-C5	5.68	108.07	105.80
55	B8	6	A	N9-C4-C5	5.68	108.07	105.80
1	AA	816	A	N3-C4-N9	5.68	131.95	127.40
22	BA	241	A	C4-C5-C6	5.68	119.84	117.00
22	BA	430	A	N3-C4-N9	5.68	131.95	127.40
22	BA	1073	A	C5-N7-C8	5.68	106.74	103.90
1	AA	807	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1150	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1152	A	C5-C6-N1	5.68	120.54	117.70
22	BA	391	A	C8-N9-C4	5.68	108.07	105.80
22	BA	2117	A	C8-N9-C4	5.68	108.07	105.80
22	BA	2211	A	C4-C5-C6	5.68	119.84	117.00
1	AA	344	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	459	A	C8-N9-C4	5.68	108.07	105.80
1	AA	759	A	N9-C4-C5	5.68	108.07	105.80
1	AA	959	A	N9-C4-C5	5.68	108.07	105.80
1	AA	1042	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1394	A	N3-C4-N9	5.68	131.94	127.40
22	BA	299	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1105	A	C4-C5-C6	5.67	119.84	117.00
22	BA	2042	A	C5-C6-N1	5.67	120.54	117.70
22	BA	2317	A	N9-C4-C5	5.67	108.07	105.80
22	BA	161	A	C4-C5-C6	5.67	119.84	117.00
22	BA	2572	A	N9-C4-C5	5.67	108.07	105.80
1	AA	306	A	C4-C5-C6	5.67	119.84	117.00
1	AA	574	A	C4-C5-C6	5.67	119.84	117.00
22	BA	282	A	C4-C5-C6	5.67	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1050	A	C5-C6-N1	5.67	120.53	117.70
22	BA	2781	A	C5-N7-C8	5.67	106.74	103.90
22	BA	2882	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	33	A	N3-C4-N9	5.67	131.94	127.40
1	AA	547	A	C4-C5-C6	5.67	119.83	117.00
22	BA	1312	U	N3-C4-O4	-5.67	115.43	119.40
22	BA	1848	A	N9-C4-C5	5.67	108.07	105.80
22	BA	56	A	C4-C5-C6	5.67	119.83	117.00
22	BA	633	A	C8-N9-C4	5.67	108.07	105.80
22	BA	1265	A	C5-N7-C8	5.67	106.73	103.90
22	BA	2660	A	N3-C4-N9	5.67	131.94	127.40
22	BA	2741	A	C4-C5-C6	5.67	119.83	117.00
23	BB	15	A	N9-C4-C5	5.67	108.07	105.80
1	AA	460	A	N3-C4-N9	5.67	131.93	127.40
22	BA	1077	A	N3-C4-N9	5.67	131.93	127.40
1	AA	1398	A	C5-C6-N1	5.66	120.53	117.70
22	BA	1342	A	C8-N9-C4	5.66	108.06	105.80
22	BA	1829	A	C5-C6-N1	5.66	120.53	117.70
22	BA	2778	A	C4-C5-N7	-5.66	107.87	110.70
1	AA	8	A	N3-C4-N9	5.66	131.93	127.40
1	AA	1319	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1885	A	C8-N9-C4	5.66	108.06	105.80
1	AA	151	A	N9-C4-C5	5.66	108.06	105.80
1	AA	496	A	C4-C5-C6	5.66	119.83	117.00
23	BB	24	G	C6-N1-C2	-5.66	121.70	125.10
22	BA	1155	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2872	A	C4-C5-C6	5.66	119.83	117.00
22	BA	528	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1635	A	C8-N9-C4	5.66	108.06	105.80
22	BA	2173	A	C4-C5-C6	5.66	119.83	117.00
22	BA	2511	U	N1-C2-N3	5.66	118.29	114.90
23	BB	59	A	C5-C6-N6	5.66	128.22	123.70
1	AA	1357	A	C5-C6-N1	5.65	120.53	117.70
22	BA	1085	A	C5-C6-N1	5.65	120.53	117.70
23	BB	115	A	C4-C5-C6	5.65	119.83	117.00
1	AA	958	A	C4-C5-N7	-5.65	107.87	110.70
22	BA	2435	A	C5-C6-N1	5.65	120.53	117.70
1	AA	572	A	N9-C4-C5	5.65	108.06	105.80
22	BA	528	A	N3-C4-N9	5.65	131.92	127.40
22	BA	821	A	N9-C4-C5	5.65	108.06	105.80
22	BA	1378	A	N9-C4-C5	5.65	108.06	105.80
22	BA	2388	A	C4-C5-N7	-5.65	107.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2443	C	C6-N1-C2	-5.65	118.04	120.30
22	BA	2513	A	C5-C6-N1	5.65	120.53	117.70
22	BA	2799	A	C5-C6-N1	5.65	120.53	117.70
1	AA	753	A	N3-C4-N9	5.65	131.92	127.40
22	BA	94	A	C8-N9-C4	5.65	108.06	105.80
1	AA	120	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1096	A	N9-C4-C5	5.65	108.06	105.80
22	BA	1664	A	C8-N9-C4	5.65	108.06	105.80
22	BA	2006	C	N1-C2-O2	5.65	122.29	118.90
1	AA	946	A	C5-C6-N1	5.65	120.52	117.70
22	BA	1321	A	C5-C6-N1	5.65	120.52	117.70
22	BA	2860	A	C8-N9-C4	5.65	108.06	105.80
1	AA	298	A	C4-C5-C6	5.64	119.82	117.00
1	AA	349	A	C5-C6-N1	5.64	120.52	117.70
1	AA	460	A	N9-C4-C5	5.64	108.06	105.80
1	AA	747	A	N9-C4-C5	5.64	108.06	105.80
1	AA	1044	A	C8-N9-C4	5.64	108.06	105.80
22	BA	789	A	C4-C5-C6	5.64	119.82	117.00
22	BA	959	A	C5-N7-C8	5.64	106.72	103.90
22	BA	1378	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2247	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2327	A	C5-C6-N1	5.64	120.52	117.70
23	BB	119	A	N3-C4-N9	5.64	131.92	127.40
1	AA	189	A	N3-C4-N9	5.64	131.91	127.40
1	AA	782	A	C4-C5-C6	5.64	119.82	117.00
22	BA	332	A	N3-C4-N9	5.64	131.91	127.40
22	BA	1014	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	1590	A	C8-N9-C4	5.64	108.06	105.80
22	BA	2327	A	C8-N9-C4	5.64	108.06	105.80
22	BA	429	A	N3-C4-N9	5.64	131.91	127.40
1	AA	787	A	N3-C4-N9	5.64	131.91	127.40
1	AA	1252	A	C5-C6-N1	5.64	120.52	117.70
22	BA	205	G	O4'-C1'-N9	5.64	112.71	108.20
22	BA	1151	A	C5-C6-N1	5.64	120.52	117.70
22	BA	1495	A	C8-N9-C4	5.64	108.06	105.80
22	BA	2266	A	C5-N7-C8	5.64	106.72	103.90
22	BA	2270	A	C4-C5-C6	5.64	119.82	117.00
55	B8	38	A	N9-C4-C5	5.64	108.06	105.80
1	AA	681	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1433	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2346	A	C8-N9-C4	5.64	108.06	105.80
22	BA	2358	A	C5-C6-N1	5.64	120.52	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	108	A	N9-C4-C5	5.64	108.06	105.80
1	AA	729	A	C4-C5-C6	5.64	119.82	117.00
1	AA	1035	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	1111	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2734	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	919	A	N9-C4-C5	5.63	108.05	105.80
1	AA	1216	A	N3-C4-N9	5.63	131.91	127.40
1	AA	1274	A	N3-C4-N9	5.63	131.91	127.40
22	BA	457	A	C4-C5-N7	-5.63	107.88	110.70
1	AA	356	A	C5-C6-N1	5.63	120.52	117.70
22	BA	1413	A	C4-C5-C6	5.63	119.82	117.00
22	BA	347	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1095	A	C4-C5-C6	5.63	119.82	117.00
22	BA	1165	A	C5-C6-N1	5.63	120.52	117.70
22	BA	1284	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1640	A	C4-C5-N7	-5.63	107.89	110.70
45	BX	33	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	AA	819	A	C8-N9-C4	5.63	108.05	105.80
1	AA	889	A	C4-C5-N7	-5.63	107.89	110.70
22	BA	1413	A	N3-C4-N9	5.63	131.90	127.40
1	AA	10	A	C5-C6-N1	5.63	120.51	117.70
1	AA	371	A	N3-C4-N9	5.63	131.90	127.40
1	AA	451	A	N9-C4-C5	5.63	108.05	105.80
1	AA	1246	A	C4-C5-C6	5.63	119.81	117.00
22	BA	346	A	N3-C4-N9	5.63	131.90	127.40
22	BA	739	A	C8-N9-C4	5.63	108.05	105.80
22	BA	1096	A	C4-C5-C6	5.63	119.81	117.00
22	BA	1286	A	N9-C4-C5	5.63	108.05	105.80
22	BA	2281	A	C5-C6-N1	5.63	120.51	117.70
22	BA	227	A	C4-C5-C6	5.63	119.81	117.00
22	BA	294	A	N3-C4-N9	5.63	131.90	127.40
22	BA	670	A	C8-N9-C4	5.63	108.05	105.80
1	AA	98	A	C5-C6-N1	5.62	120.51	117.70
1	AA	1179	A	C8-N9-C4	5.62	108.05	105.80
22	BA	1050	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	1819	A	C5-C6-N1	5.62	120.51	117.70
1	AA	831	A	N3-C4-N9	5.62	131.90	127.40
22	BA	675	A	C4-C5-C6	5.62	119.81	117.00
1	AA	1171	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1319	A	C4-C5-C6	5.62	119.81	117.00
22	BA	19	A	C5-C6-N1	5.62	120.51	117.70
22	BA	2542	A	C4-C5-N7	-5.62	107.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	600	A	N3-C4-N9	5.62	131.90	127.40
22	BA	721	A	C4-C5-C6	5.62	119.81	117.00
22	BA	861	A	N3-C4-N9	5.62	131.90	127.40
22	BA	1133	A	N3-C4-N9	5.62	131.90	127.40
22	BA	2009	A	C8-N9-C4	5.62	108.05	105.80
1	AA	109	A	N9-C4-C5	5.62	108.05	105.80
1	AA	648	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1092	A	C8-N9-C4	5.62	108.05	105.80
22	BA	42	A	C4-C5-C6	5.62	119.81	117.00
22	BA	821	A	C8-N9-C4	5.62	108.05	105.80
22	BA	972	A	C5-N7-C8	5.62	106.71	103.90
22	BA	1126	A	C5-C6-N1	5.62	120.51	117.70
22	BA	1285	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2706	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2851	A	C4-C5-C6	5.62	119.81	117.00
23	BB	39	A	N9-C4-C5	5.62	108.05	105.80
1	AA	1081	A	C5-C6-N1	5.62	120.51	117.70
22	BA	2856	A	N3-C4-N9	5.62	131.89	127.40
22	BA	199	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	478	A	N9-C4-C5	5.62	108.05	105.80
22	BA	1205	A	N3-C4-N9	5.62	131.89	127.40
22	BA	1237	A	N3-C4-N9	5.62	131.89	127.40
55	B8	51	A	C8-N9-C4	5.62	108.05	105.80
22	BA	512	G	C8-N9-C1'	5.61	134.30	127.00
22	BA	973	A	C5-N7-C8	5.61	106.71	103.90
22	BA	2736	A	C4-C5-C6	5.61	119.81	117.00
22	BA	2758	A	C4-C5-C6	5.61	119.81	117.00
1	AA	547	A	N3-C4-N9	5.61	131.89	127.40
22	BA	443	A	C5-C6-N1	5.61	120.50	117.70
22	BA	614	A	N3-C4-N9	5.61	131.89	127.40
22	BA	1169	A	C5-C6-N1	5.61	120.50	117.70
22	BA	1655	A	C4-C5-C6	5.61	119.81	117.00
1	AA	502	A	N3-C4-N9	5.61	131.89	127.40
1	AA	753	A	C5-C6-N1	5.61	120.50	117.70
1	AA	968	A	C8-N9-C4	5.61	108.04	105.80
22	BA	207	A	C4-C5-C6	5.61	119.81	117.00
22	BA	412	A	C4-C5-N7	-5.61	107.90	110.70
22	BA	2856	A	C4-C5-C6	5.61	119.81	117.00
1	AA	382	A	C8-N9-C4	5.61	108.04	105.80
1	AA	1146	A	C8-N9-C4	5.61	108.04	105.80
22	BA	165	A	C8-N9-C4	5.61	108.04	105.80
22	BA	655	A	C4-C5-N7	-5.61	107.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	676	A	C5-C6-N1	5.61	120.50	117.70
22	BA	861	A	C4-C5-C6	5.61	119.80	117.00
22	BA	1126	A	N9-C4-C5	5.61	108.04	105.80
22	BA	807	U	C5-C6-N1	-5.61	119.90	122.70
22	BA	1089	A	C5-C6-N1	5.61	120.50	117.70
22	BA	1395	A	C4-C5-C6	5.61	119.80	117.00
22	BA	1700	A	C5-C6-N1	5.61	120.50	117.70
22	BA	1890	A	C4-C5-C6	5.61	119.80	117.00
1	AA	129	A	N9-C4-C5	5.60	108.04	105.80
22	BA	582	A	C5-C6-N1	5.60	120.50	117.70
22	BA	2352	A	N3-C4-N9	5.60	131.88	127.40
1	AA	7	A	C4-C5-C6	5.60	119.80	117.00
1	AA	60	A	N3-C4-N9	5.60	131.88	127.40
1	AA	66	A	C8-N9-C4	5.60	108.04	105.80
22	BA	718	A	N3-C4-N9	5.60	131.88	127.40
22	BA	2566	A	C5-C6-N1	5.60	120.50	117.70
1	AA	767	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1288	A	C8-N9-C4	5.60	108.04	105.80
1	AA	559	A	N9-C4-C5	5.60	108.04	105.80
22	BA	354	A	C4-C5-C6	5.60	119.80	117.00
22	BA	1392	A	N3-C4-N9	5.60	131.88	127.40
22	BA	1632	A	C4-C5-C6	5.60	119.80	117.00
22	BA	1968	G	N9-C4-C5	-5.60	103.16	105.40
22	BA	2028	U	N3-C2-O2	-5.60	118.28	122.20
1	AA	344	A	C4-C5-C6	5.60	119.80	117.00
22	BA	384	A	C8-N9-C4	5.60	108.04	105.80
22	BA	788	A	C4-C5-C6	5.60	119.80	117.00
22	BA	2198	A	C8-N9-C4	5.60	108.04	105.80
23	BB	78	A	N9-C4-C5	5.60	108.04	105.80
1	AA	7	A	C8-N9-C4	5.59	108.04	105.80
1	AA	865	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	1014	A	C5-C6-N1	5.59	120.50	117.70
22	BA	1098	A	C4-C5-C6	5.59	119.80	117.00
22	BA	2158	A	N9-C4-C5	5.59	108.04	105.80
55	B8	75	C	OP1-P-OP2	5.59	127.99	119.60
1	AA	595	A	C8-N9-C4	5.59	108.04	105.80
22	BA	2778	A	N9-C4-C5	5.59	108.04	105.80
22	BA	346	A	C8-N9-C4	5.59	108.04	105.80
22	BA	800	A	C8-N9-C4	5.59	108.04	105.80
22	BA	1264	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1268	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1302	A	C4-C5-C6	5.59	119.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2530	A	C4-C5-C6	5.59	119.80	117.00
22	BA	721	A	C5-C6-N1	5.59	120.49	117.70
22	BA	2856	A	C5-C6-N1	5.59	120.49	117.70
1	AA	2	A	C4-C5-C6	5.59	119.79	117.00
22	BA	322	A	C4-C5-N7	-5.59	107.91	110.70
22	BA	844	A	N9-C4-C5	5.59	108.03	105.80
22	BA	1373	A	C8-N9-C4	5.59	108.03	105.80
22	BA	2170	A	N3-C4-N9	5.59	131.87	127.40
22	BA	2205	A	C5-C6-N1	5.59	120.49	117.70
22	BA	2482	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1392	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2126	A	N3-C4-N9	5.58	131.87	127.40
1	AA	68	G	N1-C6-O6	5.58	123.25	119.90
1	AA	621	A	N9-C4-C5	5.58	108.03	105.80
1	AA	782	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1171	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1431	A	N9-C4-C5	5.58	108.03	105.80
22	BA	354	A	N3-C4-N9	5.58	131.87	127.40
22	BA	632	A	C8-N9-C4	5.58	108.03	105.80
22	BA	748	G	O4'-C1'-N9	5.58	112.67	108.20
22	BA	1583	A	N3-C4-N9	5.58	131.87	127.40
22	BA	2542	A	N9-C4-C5	5.58	108.03	105.80
1	AA	8	A	C5-C6-N1	5.58	120.49	117.70
1	AA	26	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1016	A	N3-C4-N9	5.58	131.87	127.40
1	AA	1446	A	N3-C4-N9	5.58	131.87	127.40
22	BA	1032	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1383	A	C8-N9-C4	5.58	108.03	105.80
22	BA	2432	A	C5-N7-C8	5.58	106.69	103.90
55	B8	42	A	N3-C4-N9	5.58	131.87	127.40
1	AA	466	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	2657	A	N3-C4-N9	5.58	131.86	127.40
22	BA	2662	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	877	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1268	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1385	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1535	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	78	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	104	A	C8-N9-C4	5.58	108.03	105.80
22	BA	2095	A	C5-C6-N1	5.58	120.49	117.70
1	AA	109	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1029	A	N3-C4-N9	5.58	131.86	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2147	A	N3-C4-N9	5.58	131.86	127.40
55	B8	6	A	C4-C5-C6	5.58	119.79	117.00
1	AA	306	A	C5-C6-N1	5.57	120.49	117.70
1	AA	919	A	N3-C4-N9	5.57	131.86	127.40
22	BA	592	A	N9-C4-C5	5.57	108.03	105.80
22	BA	668	A	C4-C5-C6	5.57	119.79	117.00
22	BA	1650	A	C5-C6-N1	5.57	120.49	117.70
22	BA	1785	A	C5-N7-C8	5.57	106.69	103.90
22	BA	1809	A	C5-C6-N1	5.57	120.49	117.70
55	B8	51	A	N3-C4-N9	5.57	131.86	127.40
1	AA	55	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	309	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	502	A	C4-C5-C6	5.57	119.79	117.00
1	AA	753	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	1005	A	N9-C4-C5	5.57	108.03	105.80
22	BA	503	A	N9-C4-C5	5.57	108.03	105.80
1	AA	478	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	1012	A	N9-C4-C5	5.57	108.03	105.80
22	BA	504	A	C8-N9-C4	5.57	108.03	105.80
22	BA	1786	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	64	G	N1-C2-N2	-5.57	111.19	116.20
1	AA	1360	A	N9-C4-C5	5.57	108.03	105.80
1	AA	1465	A	C5-C6-N1	5.57	120.48	117.70
1	AA	753	A	C4-C5-C6	5.57	119.78	117.00
22	BA	1772	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	2800	A	C4-C5-C6	5.57	119.78	117.00
1	AA	309	A	C5-C6-N1	5.56	120.48	117.70
1	AA	1346	A	N3-C4-N9	5.56	131.85	127.40
1	AA	1248	A	N9-C4-C5	5.56	108.03	105.80
22	BA	12	U	N3-C2-O2	-5.56	118.31	122.20
22	BA	161	A	N3-C4-N9	5.56	131.85	127.40
22	BA	492	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	2378	A	N3-C4-N9	5.56	131.85	127.40
1	AA	298	A	N3-C4-N9	5.56	131.85	127.40
1	AA	655	A	N9-C4-C5	5.56	108.03	105.80
1	AA	50	A	C5-C6-N1	5.56	120.48	117.70
1	AA	630	A	C5-C6-N1	5.56	120.48	117.70
1	AA	816	A	C8-N9-C4	5.56	108.02	105.80
22	BA	14	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	943	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1129	A	C4-C5-C6	5.56	119.78	117.00
22	BA	666	A	N3-C4-N9	5.56	131.84	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1503	A	N3-C4-N9	5.56	131.85	127.40
22	BA	825	A	C4-C5-C6	5.56	119.78	117.00
22	BA	1230	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1000	A	C4-C5-C6	5.55	119.78	117.00
22	BA	936	A	N3-C4-N9	5.55	131.84	127.40
22	BA	833	A	C5-N7-C8	5.55	106.68	103.90
22	BA	896	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	1126	A	N3-C4-N9	5.55	131.84	127.40
22	BA	2270	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	2311	A	N3-C4-N9	5.55	131.84	127.40
1	AA	171	A	C5-C6-N1	5.55	120.48	117.70
22	BA	541	A	N9-C4-C5	5.55	108.02	105.80
22	BA	1789	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	718	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	784	G	P-O3'-C3'	5.55	126.36	119.70
22	BA	1785	A	N3-C4-N9	5.55	131.84	127.40
22	BA	346	A	N9-C4-C5	5.55	108.02	105.80
1	AA	80	A	C8-N9-C4	5.55	108.02	105.80
1	AA	663	A	N9-C4-C5	5.55	108.02	105.80
1	AA	716	A	C5-C6-N1	5.55	120.47	117.70
1	AA	872	A	C4-C5-C6	5.55	119.77	117.00
22	BA	538	A	C5-C6-N1	5.55	120.47	117.70
55	B8	69	A	C5-C6-N1	5.55	120.47	117.70
1	AA	640	A	C4-C5-C6	5.54	119.77	117.00
1	AA	1111	A	N9-C4-C5	5.54	108.02	105.80
22	BA	125	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	223	A	N3-C4-N9	5.54	131.83	127.40
22	BA	739	A	C4-C5-C6	5.54	119.77	117.00
22	BA	896	A	N9-C4-C5	5.54	108.02	105.80
22	BA	984	A	N9-C4-C5	5.54	108.02	105.80
22	BA	1665	A	N3-C4-N9	5.54	131.84	127.40
22	BA	2205	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	2809	A	C8-N9-C4	5.54	108.02	105.80
1	AA	344	A	N3-C4-N9	5.54	131.83	127.40
1	AA	364	A	N3-C4-N9	5.54	131.83	127.40
22	BA	2726	A	N3-C4-N9	5.54	131.83	127.40
1	AA	44	A	N3-C4-N9	5.54	131.83	127.40
1	AA	67	C	N3-C4-C5	5.54	124.12	121.90
1	AA	325	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	365	U	C2-N3-C4	5.54	130.32	127.00
22	BA	1544	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	2346	A	C4-C5-N7	-5.54	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1250	A	N3-C4-N9	5.54	131.83	127.40
22	BA	270	A	C4-C5-C6	5.54	119.77	117.00
22	BA	2009	A	C4-C5-C6	5.54	119.77	117.00
1	AA	499	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	600	A	C4-C5-C6	5.54	119.77	117.00
1	AA	1042	A	N3-C4-N9	5.54	131.83	127.40
22	BA	761	A	C8-N9-C4	5.54	108.01	105.80
22	BA	2134	A	C4-C5-C6	5.54	119.77	117.00
22	BA	218	A	C4-C5-C6	5.53	119.77	117.00
22	BA	278	A	N9-C4-C5	5.53	108.01	105.80
22	BA	429	A	N9-C4-C5	5.53	108.01	105.80
55	B8	58	A	N3-C4-N9	5.53	131.83	127.40
1	AA	607	A	N9-C4-C5	5.53	108.01	105.80
1	AA	640	A	N3-C4-N9	5.53	131.82	127.40
1	AA	1219	A	C5-C6-N1	5.53	120.47	117.70
22	BA	661	A	N3-C4-N9	5.53	131.83	127.40
1	AA	160	A	C8-N9-C4	5.53	108.01	105.80
1	AA	313	A	C5-C6-N1	5.53	120.47	117.70
1	AA	872	A	C5-C6-N1	5.53	120.47	117.70
1	AA	1101	A	C4-C5-N7	-5.53	107.93	110.70
22	BA	294	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	1322	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1383	A	C5-C6-N1	5.53	120.47	117.70
22	BA	1495	A	C4-C5-C6	5.53	119.77	117.00
22	BA	2530	A	N3-C4-N9	5.53	131.82	127.40
22	BA	2883	A	N3-C4-N9	5.53	131.82	127.40
1	AA	129	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	1916	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	1928	A	N3-C4-N9	5.53	131.82	127.40
1	AA	969	A	N3-C4-N9	5.53	131.82	127.40
22	BA	1186	G	O5'-P-OP1	-5.53	100.73	105.70
22	BA	1522	A	N9-C4-C5	5.53	108.01	105.80
1	AA	547	A	C5-C6-N1	5.53	120.46	117.70
1	AA	759	A	C5-C6-N1	5.53	120.46	117.70
1	AA	900	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1362	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	637	A	N3-C4-N9	5.53	131.82	127.40
22	BA	699	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1580	A	N3-C4-N9	5.53	131.82	127.40
1	AA	151	A	C5-C6-N1	5.52	120.46	117.70
1	AA	919	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1531	A	N9-C4-C5	5.52	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	941	A	C5-N7-C8	5.52	106.66	103.90
22	BA	2882	A	N9-C4-C5	5.52	108.01	105.80
22	BA	972	A	C5-C6-N1	5.52	120.46	117.70
22	BA	1088	A	C5-C6-N1	5.52	120.46	117.70
22	BA	1701	A	C5-C6-N1	5.52	120.46	117.70
23	BB	34	A	C5-C6-N1	5.52	120.46	117.70
55	B8	38	A	C4-C5-C6	5.52	119.76	117.00
22	BA	1069	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1431	A	C4-C5-C6	5.52	119.76	117.00
22	BA	2887	A	C8-N9-C4	5.52	108.01	105.80
22	BA	2900	A	C5-C6-N1	5.52	120.46	117.70
1	AA	935	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1289	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1515	A	C4-C5-C6	5.52	119.76	117.00
22	BA	1598	A	N9-C4-C5	5.52	108.01	105.80
22	BA	2274	A	C8-N9-C4	5.52	108.01	105.80
1	AA	119	A	N3-C4-N9	5.52	131.81	127.40
1	AA	155	A	C4-C5-C6	5.52	119.76	117.00
1	AA	1251	A	C8-N9-C4	5.52	108.01	105.80
22	BA	320	A	N3-C4-N9	5.52	131.81	127.40
22	BA	2088	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2564	A	C5-C6-N1	5.52	120.46	117.70
22	BA	118	A	C4-C5-C6	5.51	119.76	117.00
22	BA	1566	A	N3-C4-N9	5.51	131.81	127.40
1	AA	373	A	C4-C5-C6	5.51	119.75	117.00
1	AA	1447	A	N3-C4-N9	5.51	131.81	127.40
22	BA	104	A	C5-C6-N1	5.51	120.45	117.70
22	BA	743	A	C4-C5-C6	5.51	119.76	117.00
22	BA	1336	A	C5-C6-N1	5.51	120.45	117.70
22	BA	1403	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	1509	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	1739	A	N9-C4-C5	5.51	108.00	105.80
22	BA	1789	A	N9-C4-C5	5.51	108.00	105.80
22	BA	2376	A	N3-C4-N9	5.51	131.81	127.40
22	BA	2467	C	N3-C4-C5	5.51	124.11	121.90
1	AA	1105	A	C5-C6-N1	5.51	120.45	117.70
22	BA	2753	A	C8-N9-C4	5.51	108.00	105.80
1	AA	315	A	N3-C4-N9	5.51	131.81	127.40
1	AA	1204	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	1271	A	C4-C5-C6	5.51	119.75	117.00
1	AA	1280	A	C5-C6-N1	5.51	120.45	117.70
1	AA	1333	A	C5-C6-N1	5.51	120.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1465	A	C4-C5-C6	5.51	119.75	117.00
22	BA	347	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	938	A	N9-C4-C5	5.50	108.00	105.80
22	BA	1821	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	55	A	N9-C4-C5	5.50	108.00	105.80
1	AA	152	A	C5-C6-N1	5.50	120.45	117.70
1	AA	179	A	C8-N9-C4	5.50	108.00	105.80
1	AA	263	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	715	A	C4-C5-C6	5.50	119.75	117.00
22	BA	866	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1890	A	N9-C4-C5	5.50	108.00	105.80
22	BA	2665	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	262	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1096	A	C5-C6-N1	5.50	120.45	117.70
1	AA	1502	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1532	A	N3-C4-N9	5.50	131.80	127.40
1	AA	510	A	C4-C5-C6	5.50	119.75	117.00
1	AA	706	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1157	A	C5-C6-N1	5.50	120.45	117.70
22	BA	457	A	N9-C4-C5	5.50	108.00	105.80
22	BA	602	A	C4-C5-C6	5.50	119.75	117.00
1	AA	1130	A	N3-C4-N9	5.50	131.80	127.40
22	BA	609	A	C5-C6-N1	5.50	120.45	117.70
22	BA	2108	A	N9-C4-C5	5.50	108.00	105.80
22	BA	2748	A	N3-C4-N9	5.50	131.80	127.40
1	AA	1398	A	N3-C4-N9	5.49	131.79	127.40
22	BA	541	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2761	A	C8-N9-C4	5.49	108.00	105.80
22	BA	466	A	C4-C5-C6	5.49	119.75	117.00
1	AA	374	A	C5-C6-N1	5.49	120.45	117.70
1	AA	787	A	C5-C6-N1	5.49	120.44	117.70
22	BA	1690	A	C4-C5-N7	-5.49	107.95	110.70
22	BA	2297	A	C8-N9-C4	5.49	108.00	105.80
22	BA	2471	A	C4-C5-N7	-5.49	107.95	110.70
22	BA	2572	A	C4-C5-C6	5.49	119.75	117.00
22	BA	2809	A	C5-C6-N1	5.49	120.44	117.70
1	AA	373	A	C5-C6-N1	5.49	120.44	117.70
1	AA	411	A	C4-C5-C6	5.49	119.74	117.00
1	AA	996	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2426	A	C8-N9-C4	5.49	108.00	105.80
22	BA	2590	A	C5-C6-N1	5.49	120.44	117.70
1	AA	1	A	C5-C6-N1	5.49	120.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	197	A	C4-C5-C6	5.49	119.74	117.00
1	AA	1251	A	C5-C6-N1	5.49	120.44	117.70
22	BA	217	A	N3-C4-N9	5.49	131.79	127.40
22	BA	502	A	C4-C5-C6	5.49	119.74	117.00
22	BA	1889	A	C8-N9-C4	5.49	107.99	105.80
22	BA	2097	A	C8-N9-C4	5.49	108.00	105.80
1	AA	26	A	N3-C4-N9	5.48	131.79	127.40
22	BA	126	A	C8-N9-C4	5.48	107.99	105.80
22	BA	1327	A	N3-C4-N9	5.48	131.78	127.40
22	BA	2126	A	C4-C5-C6	5.48	119.74	117.00
22	BA	2317	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	81	A	N9-C4-C5	5.48	107.99	105.80
1	AA	282	A	N9-C4-C5	5.48	107.99	105.80
22	BA	515	A	C5-C6-N1	5.48	120.44	117.70
22	BA	613	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2449	U	C6-N1-C2	5.48	124.29	121.00
1	AA	451	A	C5-C6-N1	5.48	120.44	117.70
22	BA	6	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1130	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1274	A	C8-N9-C4	5.48	107.99	105.80
22	BA	479	A	C4-C5-C6	5.48	119.74	117.00
22	BA	792	A	N9-C4-C5	5.48	107.99	105.80
22	BA	979	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	1593	A	C5-C6-N1	5.48	120.44	117.70
22	BA	1801	A	C8-N9-C4	5.48	107.99	105.80
22	BA	2660	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	553	A	C5-C6-N1	5.47	120.44	117.70
22	BA	195	A	N3-C4-N9	5.47	131.78	127.40
22	BA	1876	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	2173	A	N9-C4-C5	5.47	107.99	105.80
23	BB	104	A	C8-N9-C4	5.47	107.99	105.80
22	BA	244	A	C4-C5-C6	5.47	119.74	117.00
22	BA	547	A	N9-C4-C5	5.47	107.99	105.80
22	BA	346	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	179	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	1145	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	44	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	432	A	C4-C5-C6	5.47	119.73	117.00
22	BA	483	A	C8-N9-C4	5.47	107.99	105.80
22	BA	1672	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2297	A	N3-C4-N9	5.47	131.78	127.40
22	BA	1739	A	C5-N7-C8	5.47	106.63	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1509	A	N3-C4-N9	5.47	131.77	127.40
55	B8	41	A	C8-N9-C4	5.47	107.99	105.80
22	BA	980	A	C8-N9-C4	5.46	107.99	105.80
22	BA	1987	A	C5-C6-N1	5.46	120.43	117.70
22	BA	1515	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1755	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1936	A	N9-C4-C5	5.46	107.98	105.80
1	AA	510	A	N3-C4-N9	5.46	131.77	127.40
1	AA	1480	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	866	A	C5-C6-N1	5.46	120.43	117.70
22	BA	1689	A	C8-N9-C4	5.46	107.98	105.80
22	BA	1744	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	1966	A	C8-N9-C4	5.46	107.98	105.80
22	BA	2547	A	N3-C4-N9	5.46	131.77	127.40
1	AA	574	A	C8-N9-C4	5.46	107.98	105.80
1	AA	777	A	C8-N9-C4	5.46	107.98	105.80
1	AA	787	A	C4-C5-C6	5.46	119.73	117.00
22	BA	144	A	C4-C5-C6	5.46	119.73	117.00
22	BA	191	A	N3-C4-N9	5.46	131.77	127.40
22	BA	324	A	C4-C5-C6	5.46	119.73	117.00
22	BA	2377	A	C5-C6-N1	5.46	120.43	117.70
22	BA	2392	A	N9-C4-C5	5.46	107.98	105.80
1	AA	397	A	N9-C4-C5	5.46	107.98	105.80
1	AA	815	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	1494	A	N9-C4-C5	5.46	107.98	105.80
1	AA	949	A	C8-N9-C4	5.46	107.98	105.80
1	AA	1163	A	N3-C4-N9	5.46	131.76	127.40
1	AA	77	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	621	A	C4-C5-C6	5.45	119.73	117.00
1	AA	1110	A	N3-C4-N9	5.45	131.76	127.40
1	AA	1500	A	C5-C6-N1	5.45	120.43	117.70
22	BA	14	A	C4-C5-C6	5.45	119.73	117.00
22	BA	71	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	165	A	N9-C4-C5	5.45	107.98	105.80
22	BA	2028	U	N1-C2-O2	5.45	126.62	122.80
22	BA	2274	A	C5-C6-N1	5.45	120.43	117.70
22	BA	342	A	N3-C4-N9	5.45	131.76	127.40
22	BA	1794	A	N3-C4-N9	5.45	131.76	127.40
55	B8	21	A	C4-C5-C6	5.45	119.73	117.00
1	AA	1000	A	C5-C6-N1	5.45	120.42	117.70
22	BA	1142	A	C5-C6-N1	5.45	120.42	117.70
22	BA	2163	A	C4-C5-C6	5.45	119.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	144	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	1285	A	C5-C6-N1	5.45	120.42	117.70
23	BB	94	A	C5-C6-N1	5.45	120.42	117.70
1	AA	1340	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	563	A	C5-C6-N1	5.45	120.42	117.70
22	BA	1327	A	C5-C6-N1	5.44	120.42	117.70
22	BA	2635	A	N9-C4-C5	5.44	107.98	105.80
1	AA	695	A	C4-C5-C6	5.44	119.72	117.00
1	AA	1271	A	N3-C4-N9	5.44	131.75	127.40
22	BA	142	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	142	A	C8-N9-C4	5.44	107.98	105.80
22	BA	2761	A	N9-C4-C5	5.44	107.98	105.80
22	BA	2660	A	C8-N9-C4	5.44	107.98	105.80
1	AA	1101	A	C4-C5-C6	5.44	119.72	117.00
1	AA	1410	A	C4-C5-C6	5.44	119.72	117.00
22	BA	94	A	C4-C5-C6	5.44	119.72	117.00
22	BA	472	A	C8-N9-C4	5.44	107.98	105.80
22	BA	1571	A	C8-N9-C4	5.44	107.98	105.80
22	BA	1010	A	C4-C5-C6	5.44	119.72	117.00
22	BA	2311	A	C5-C6-N1	5.44	120.42	117.70
22	BA	1593	A	C4-C5-C6	5.44	119.72	117.00
23	BB	29	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	181	A	C4-C5-C6	5.43	119.72	117.00
1	AA	702	A	N9-C4-C5	5.43	107.97	105.80
1	AA	787	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1019	A	C8-N9-C4	5.43	107.97	105.80
22	BA	222	A	C4-C5-C6	5.43	119.72	117.00
22	BA	1701	A	C8-N9-C4	5.43	107.97	105.80
1	AA	303	A	C4-C5-C6	5.43	119.72	117.00
1	AA	1036	A	C4-C5-C6	5.43	119.72	117.00
1	AA	1476	A	N3-C4-N9	5.43	131.75	127.40
22	BA	1785	A	N9-C4-C5	5.43	107.97	105.80
1	AA	129	A	N3-C4-N9	5.43	131.75	127.40
1	AA	236	A	C5-C6-N1	5.43	120.42	117.70
1	AA	825	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	50	A	N9-C4-C5	5.43	107.97	105.80
1	AA	509	A	C5-C6-N1	5.43	120.42	117.70
1	AA	1319	A	N3-C4-N9	5.43	131.74	127.40
1	AA	1410	A	C8-N9-C4	5.43	107.97	105.80
22	BA	6	A	C8-N9-C4	5.43	107.97	105.80
22	BA	221	A	C5-C6-N1	5.43	120.42	117.70
22	BA	706	A	C4-C5-N7	-5.43	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1786	A	C5-C6-N1	5.43	120.42	117.70
22	BA	2726	A	C5-C6-N1	5.43	120.42	117.70
55	B8	21	A	N3-C4-N9	5.43	131.74	127.40
22	BA	613	A	C4-C5-N7	-5.43	107.99	110.70
23	BB	94	A	N9-C4-C5	5.43	107.97	105.80
1	AA	51	A	N3-C4-N9	5.43	131.74	127.40
1	AA	171	A	N9-C4-C5	5.43	107.97	105.80
1	AA	704	A	N3-C4-N9	5.43	131.74	127.40
22	BA	2095	A	C8-N9-C4	5.43	107.97	105.80
22	BA	2189	U	N1-C2-O2	-5.43	119.00	122.80
22	BA	165	A	N3-C4-N9	5.42	131.74	127.40
22	BA	1076	C	N1-C2-O2	5.42	122.16	118.90
22	BA	1552	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1360	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	1515	A	C8-N9-C4	5.42	107.97	105.80
1	AA	431	A	C4-C5-C6	5.42	119.71	117.00
22	BA	262	A	C4-C5-C6	5.42	119.71	117.00
22	BA	515	A	N3-C4-N9	5.42	131.74	127.40
22	BA	716	A	N3-C4-N9	5.42	131.74	127.40
22	BA	2425	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	423	A	C5-C6-N1	5.42	120.41	117.70
22	BA	1427	A	C5-C6-N1	5.42	120.41	117.70
1	AA	205	A	C5-C6-N1	5.42	120.41	117.70
1	AA	250	A	C4-C5-C6	5.42	119.71	117.00
1	AA	412	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1503	A	C4-C5-C6	5.42	119.71	117.00
22	BA	1028	A	C5-C6-N1	5.42	120.41	117.70
22	BA	1635	A	N3-C4-N9	5.42	131.74	127.40
22	BA	2358	A	N3-C4-N9	5.42	131.74	127.40
22	BA	310	A	N3-C4-N9	5.42	131.73	127.40
22	BA	432	A	N3-C4-N9	5.42	131.73	127.40
22	BA	1525	A	C4-C5-C6	5.42	119.71	117.00
22	BA	2376	A	C4-C5-C6	5.42	119.71	117.00
22	BA	2721	A	C5-C6-N1	5.42	120.41	117.70
23	BB	115	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	917	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2147	A	C4-C5-C6	5.42	119.71	117.00
1	AA	139	A	N9-C4-C5	5.41	107.97	105.80
1	AA	919	A	C5-C6-N1	5.41	120.41	117.70
1	AA	1257	A	C4-C5-N7	-5.41	107.99	110.70
22	BA	1609	A	C5-C6-N1	5.41	120.41	117.70
22	BA	2031	A	C5-C6-N1	5.41	120.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	14	A	N9-C4-C5	5.41	107.97	105.80
1	AA	161	A	C5-C6-N1	5.41	120.41	117.70
1	AA	412	A	C4-C5-C6	5.41	119.71	117.00
22	BA	332	A	C5-C6-N1	5.41	120.41	117.70
22	BA	513	A	C5-C6-N1	5.41	120.41	117.70
1	AA	197	A	N3-C4-N9	5.41	131.73	127.40
1	AA	382	A	N3-C4-N9	5.41	131.73	127.40
1	AA	600	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	864	A	N9-C4-C5	5.41	107.97	105.80
22	BA	470	A	N9-C4-C5	5.41	107.96	105.80
22	BA	800	A	C6-N1-C2	5.41	121.85	118.60
1	AA	728	A	N9-C4-C5	5.41	107.96	105.80
1	AA	994	A	C5-C6-N1	5.41	120.41	117.70
22	BA	928	A	C5-C6-N1	5.41	120.40	117.70
22	BA	1525	A	N3-C4-N9	5.41	131.73	127.40
22	BA	1655	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	2765	A	C5-C6-N1	5.41	120.41	117.70
22	BA	19	A	C8-N9-C4	5.41	107.96	105.80
22	BA	1046	A	N3-C4-N9	5.41	131.72	127.40
1	AA	253	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	364	A	C5-C6-N1	5.41	120.40	117.70
22	BA	1899	A	C8-N9-C4	5.41	107.96	105.80
1	AA	777	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	1749	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	918	A	C4-C5-C6	5.40	119.70	117.00
22	BA	2088	A	N9-C4-C5	5.40	107.96	105.80
22	BA	2634	A	N3-C4-N9	5.40	131.72	127.40
1	AA	33	A	N9-C4-C5	5.40	107.96	105.80
1	AA	559	A	C8-N9-C4	5.40	107.96	105.80
1	AA	792	A	O4'-C1'-N9	5.40	112.52	108.20
22	BA	199	A	C8-N9-C4	5.40	107.96	105.80
22	BA	322	A	N9-C4-C5	5.40	107.96	105.80
22	BA	943	A	C5-N7-C8	5.40	106.60	103.90
22	BA	1603	A	C4-C5-C6	5.40	119.70	117.00
22	BA	1669	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	207	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	1392	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	2005	A	C5-C6-N1	5.40	120.40	117.70
1	AA	26	A	C4-C5-C6	5.40	119.70	117.00
1	AA	729	A	C5-C6-N1	5.40	120.40	117.70
22	BA	1679	A	C8-N9-C4	5.40	107.96	105.80
22	BA	2635	A	C4-C5-N7	-5.40	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2809	A	C4-C5-C6	5.40	119.70	117.00
55	B8	6	A	C8-N9-C4	5.40	107.96	105.80
55	B8	58	A	C4-C5-C6	5.40	119.70	117.00
22	BA	10	A	C5-C6-N1	5.40	120.40	117.70
22	BA	2753	A	C4-C5-N7	-5.40	108.00	110.70
55	B8	14	A	C8-N9-C4	5.40	107.96	105.80
1	AA	33	A	C8-N9-C4	5.39	107.96	105.80
1	AA	918	A	C4-C5-C6	5.39	119.70	117.00
1	AA	1146	A	N3-C4-N9	5.39	131.72	127.40
22	BA	402	A	C5-C6-N1	5.39	120.40	117.70
22	BA	1127	A	C5-C6-N1	5.39	120.40	117.70
1	AA	1176	A	C5-C6-N1	5.39	120.40	117.70
1	AA	1269	A	N3-C4-N9	5.39	131.71	127.40
22	BA	1039	A	C5-C6-N1	5.39	120.40	117.70
22	BA	1801	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1928	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	408	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1413	A	C8-N9-C4	5.39	107.96	105.80
1	AA	495	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	1419	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1966	A	C4-C5-C6	5.39	119.69	117.00
22	BA	2757	A	N9-C4-C5	5.39	107.96	105.80
55	B8	42	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	238	A	C8-N9-C4	5.39	107.95	105.80
1	AA	1431	A	C4-C5-C6	5.39	119.69	117.00
22	BA	616	A	C5-C6-N1	5.39	120.39	117.70
22	BA	1205	A	C4-C5-C6	5.39	119.69	117.00
22	BA	1808	A	N3-C4-N9	5.39	131.71	127.40
22	BA	1916	A	N3-C4-N9	5.39	131.71	127.40
1	AA	98	A	C8-N9-C4	5.38	107.95	105.80
22	BA	599	A	C8-N9-C4	5.38	107.95	105.80
22	BA	1981	A	C4-C5-C6	5.38	119.69	117.00
22	BA	2749	A	C5-N7-C8	5.38	106.59	103.90
1	AA	1105	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	592	A	C8-N9-C4	5.38	107.95	105.80
22	BA	2058	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	533	A	C5-C6-N1	5.38	120.39	117.70
1	AA	777	A	C4-C5-C6	5.38	119.69	117.00
1	AA	1362	A	N3-C4-N9	5.38	131.70	127.40
22	BA	42	A	C5-C6-N1	5.38	120.39	117.70
22	BA	532	A	N9-C4-C5	5.38	107.95	105.80
22	BA	1126	A	C4-C5-C6	5.38	119.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1545	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1229	A	N3-C4-N9	5.38	131.70	127.40
1	AA	7	A	C5-C6-N1	5.38	120.39	117.70
1	AA	1287	A	N3-C4-N9	5.38	131.70	127.40
22	BA	599	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1354	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1535	A	C5-C6-N1	5.38	120.39	117.70
22	BA	1772	A	N9-C4-C5	5.38	107.95	105.80
22	BA	2736	A	C8-N9-C4	5.38	107.95	105.80
1	AA	909	A	N3-C4-N9	5.38	131.70	127.40
1	AA	1248	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1500	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	199	A	N3-C4-N9	5.38	131.70	127.40
1	AA	382	A	C5-C6-N1	5.38	120.39	117.70
22	BA	866	A	C4-C5-C6	5.38	119.69	117.00
1	AA	53	A	C5-C6-N1	5.37	120.39	117.70
1	AA	1350	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	167	A	C5-C6-N1	5.37	120.39	117.70
22	BA	979	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1039	A	C4-C5-C6	5.37	119.69	117.00
22	BA	2227	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	2826	A	C8-N9-C4	5.37	107.95	105.80
55	B8	42	A	C5-C6-N1	5.37	120.39	117.70
1	AA	67	C	C5-C6-N1	-5.37	118.31	121.00
1	AA	608	A	C4-C5-C6	5.37	119.69	117.00
1	AA	629	A	C8-N9-C4	5.37	107.95	105.80
1	AA	1227	A	C5-N7-C8	5.37	106.58	103.90
22	BA	819	A	C5-C6-N1	5.37	120.39	117.70
22	BA	1453	A	N3-C4-N9	5.37	131.70	127.40
1	AA	382	A	N9-C4-C5	5.37	107.95	105.80
1	AA	648	A	C5-C6-N1	5.37	120.38	117.70
1	AA	1005	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	706	A	C5-C6-N1	5.37	120.38	117.70
22	BA	2418	A	C5-C6-N1	5.37	120.38	117.70
22	BA	2792	A	C8-N9-C4	5.37	107.95	105.80
1	AA	1375	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	160	A	C4-C5-C6	5.37	119.68	117.00
22	BA	191	A	N9-C4-C5	5.37	107.95	105.80
22	BA	221	A	N9-C4-C5	5.37	107.95	105.80
22	BA	675	A	C5-C6-N1	5.37	120.38	117.70
22	BA	984	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	988	A	C5-C6-N1	5.37	120.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1551	A	C5-C6-N1	5.37	120.38	117.70
22	BA	2321	U	N3-C2-O2	-5.37	118.44	122.20
1	AA	274	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	412	A	N3-C4-N9	5.36	131.69	127.40
1	AA	1493	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	344	A	N3-C4-N9	5.36	131.69	127.40
22	BA	718	A	N9-C4-C5	5.36	107.95	105.80
22	BA	2727	A	C8-N9-C4	5.36	107.95	105.80
22	BA	1367	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	83	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	2	A	N3-C4-N9	5.36	131.69	127.40
1	AA	274	A	N3-C4-N9	5.36	131.69	127.40
1	AA	382	A	C4-C5-C6	5.36	119.68	117.00
1	AA	1288	A	N3-C4-N9	5.36	131.69	127.40
22	BA	64	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	1374	A	C8-N9-C4	5.36	107.94	105.80
1	AA	1447	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2183	A	C8-N9-C4	5.36	107.94	105.80
22	BA	2284	A	C8-N9-C4	5.36	107.94	105.80
22	BA	2352	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1111	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	63	A	C4-C5-C6	5.36	119.68	117.00
22	BA	1269	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1374	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	160	A	C5-C6-N1	5.35	120.38	117.70
22	BA	1244	A	C5-C6-N1	5.35	120.38	117.70
22	BA	1937	A	C5-C6-N1	5.35	120.38	117.70
22	BA	2837	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1117	A	N3-C4-N9	5.35	131.68	127.40
1	AA	1246	A	N9-C4-C5	5.35	107.94	105.80
22	BA	204	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	512	G	N9-C4-C5	5.35	107.54	105.40
22	BA	821	A	C5-C6-N1	5.35	120.38	117.70
22	BA	2826	A	C4-C5-C6	5.35	119.68	117.00
55	B8	66	A	C8-N9-C4	5.35	107.94	105.80
1	AA	923	A	N9-C4-C5	5.35	107.94	105.80
1	AA	78	A	N3-C4-N9	5.35	131.68	127.40
1	AA	1250	A	C8-N9-C4	5.35	107.94	105.80
22	BA	734	A	C4-C5-C6	5.35	119.67	117.00
22	BA	1328	A	C4-C5-C6	5.35	119.67	117.00
22	BA	1393	A	N3-C4-N9	5.35	131.68	127.40
22	BA	1544	A	C5-C6-N1	5.35	120.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1598	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	1660	G	C5-C6-O6	5.35	131.81	128.60
22	BA	1970	A	C5-C6-N1	5.35	120.37	117.70
1	AA	648	A	N3-C4-N9	5.35	131.68	127.40
1	AA	663	A	C5-C6-N1	5.35	120.37	117.70
1	AA	746	A	C8-N9-C4	5.35	107.94	105.80
1	AA	1016	A	C5-C6-N1	5.35	120.37	117.70
1	AA	1396	A	N9-C4-C5	5.35	107.94	105.80
22	BA	428	A	C8-N9-C4	5.35	107.94	105.80
22	BA	936	A	C4-C5-C6	5.35	119.67	117.00
1	AA	161	A	C8-N9-C4	5.35	107.94	105.80
1	AA	607	A	C8-N9-C4	5.35	107.94	105.80
22	BA	38	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	1347	A	N9-C4-C5	5.34	107.94	105.80
22	BA	2482	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	250	A	N3-C4-N9	5.34	131.67	127.40
22	BA	1086	A	N3-C4-N9	5.34	131.68	127.40
22	BA	2288	A	C5-C6-N1	5.34	120.37	117.70
23	BB	53	A	N9-C4-C5	5.34	107.94	105.80
1	AA	81	A	C8-N9-C4	5.34	107.94	105.80
1	AA	1275	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	1377	A	N3-C4-N9	5.34	131.67	127.40
22	BA	792	A	C4-C5-C6	5.34	119.67	117.00
22	BA	947	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	1262	A	C5-C6-N1	5.34	120.37	117.70
22	BA	1794	A	C4-C5-C6	5.34	119.67	117.00
22	BA	1815	A	N3-C4-N9	5.34	131.67	127.40
22	BA	2067	G	N1-C6-O6	-5.34	116.70	119.90
22	BA	2071	A	C8-N9-C4	5.34	107.94	105.80
23	BB	29	A	N3-C4-N9	5.34	131.67	127.40
2	AB	204	ASP	CB-CG-OD1	-5.34	113.50	118.30
22	BA	119	A	C8-N9-C4	5.34	107.94	105.80
22	BA	430	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	590	A	C4-C5-C6	5.34	119.67	117.00
22	BA	1095	A	C8-N9-C4	5.34	107.94	105.80
22	BA	1433	A	C5-C6-N1	5.34	120.37	117.70
22	BA	1815	A	C5-C6-N1	5.34	120.37	117.70
55	B8	73	A	C4-C5-C6	5.34	119.67	117.00
1	AA	223	A	C8-N9-C4	5.34	107.94	105.80
22	BA	1677	A	C6-N1-C2	5.34	121.80	118.60
1	AA	74	A	N3-C4-N9	5.34	131.67	127.40
22	BA	1802	A	C5-N7-C8	5.34	106.57	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	78	A	C5-C6-N1	5.34	120.37	117.70
1	AA	1016	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1084	A	C8-N9-C4	5.33	107.93	105.80
1	AA	1082	A	N9-C4-C5	5.33	107.93	105.80
22	BA	666	A	C8-N9-C4	5.33	107.93	105.80
22	BA	2335	A	N9-C4-C5	5.33	107.93	105.80
22	BA	2534	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	2577	A	C8-N9-C4	5.33	107.93	105.80
1	AA	344	A	C8-N9-C4	5.33	107.93	105.80
1	AA	415	A	C8-N9-C4	5.33	107.93	105.80
1	AA	825	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1204	A	C5-C6-N1	5.33	120.37	117.70
22	BA	833	A	C4-C5-C6	5.33	119.67	117.00
22	BA	2009	A	N3-C4-N9	5.33	131.66	127.40
22	BA	2311	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	465	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1204	A	N3-C4-N9	5.33	131.66	127.40
22	BA	1254	A	O5'-P-OP1	-5.33	100.90	105.70
22	BA	2418	A	C4-C5-C6	5.33	119.67	117.00
1	AA	149	A	N3-C4-N9	5.33	131.66	127.40
1	AA	759	A	N3-C4-N9	5.33	131.66	127.40
22	BA	1614	A	C5-N7-C8	5.33	106.56	103.90
22	BA	2324	U	N1-C2-O2	5.33	126.53	122.80
22	BA	2767	C	C6-N1-C2	-5.33	118.17	120.30
36	BO	32	PRO	CA-N-CD	-5.33	104.04	111.50
22	BA	807	U	N3-C4-C5	5.33	117.80	114.60
22	BA	1420	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	1357	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	429	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	479	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	1054	A	C8-N9-C4	5.33	107.93	105.80
22	BA	1194	A	C5-C6-N1	5.33	120.36	117.70
22	BA	1785	A	C4-C5-C6	5.33	119.66	117.00
22	BA	2241	A	C8-N9-C4	5.33	107.93	105.80
22	BA	2873	A	C5-N7-C8	5.33	106.56	103.90
1	AA	649	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	1419	A	N3-C4-N9	5.32	131.66	127.40
22	BA	2439	A	N3-C4-N9	5.32	131.66	127.40
22	BA	1134	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2740	A	N3-C4-N9	5.32	131.66	127.40
1	AA	1219	A	C8-N9-C4	5.32	107.93	105.80
22	BA	227	A	N3-C4-N9	5.32	131.66	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	575	A	C4-C5-C6	5.32	119.66	117.00
22	BA	1616	A	C5-C6-N1	5.32	120.36	117.70
22	BA	2273	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	831	A	N9-C4-C5	5.32	107.93	105.80
1	AA	10	A	C4-C5-C6	5.32	119.66	117.00
22	BA	512	G	C4-N9-C1'	-5.32	119.59	126.50
22	BA	1548	A	N3-C4-N9	5.32	131.66	127.40
22	BA	2211	A	C5-C6-N1	5.32	120.36	117.70
55	B8	51	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	892	A	C8-N9-C4	5.32	107.93	105.80
22	BA	2860	A	N9-C4-C5	5.32	107.93	105.80
23	BB	53	A	C5-C6-N1	5.32	120.36	117.70
22	BA	685	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	1889	A	N9-C4-C5	5.31	107.92	105.80
22	BA	125	A	C5-C6-N1	5.31	120.36	117.70
22	BA	590	A	N9-C4-C5	5.31	107.92	105.80
22	BA	603	A	N9-C4-C5	5.31	107.92	105.80
22	BA	2837	A	C4-C5-C6	5.31	119.66	117.00
55	B8	14	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	783	A	C5-C6-N1	5.31	120.36	117.70
1	AA	554	A	C5-C6-N1	5.31	120.35	117.70
22	BA	751	A	C8-N9-C4	5.31	107.92	105.80
22	BA	1772	A	N3-C4-N9	5.31	131.65	127.40
1	AA	1254	A	C5-C6-N1	5.31	120.35	117.70
22	BA	311	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	311	A	N3-C4-N9	5.31	131.65	127.40
22	BA	478	A	C5-C6-N1	5.31	120.35	117.70
22	BA	1919	A	N3-C4-N9	5.31	131.65	127.40
22	BA	2134	A	N3-C4-N9	5.31	131.65	127.40
1	AA	595	A	C5-C6-N1	5.31	120.35	117.70
1	AA	766	A	N3-C4-N9	5.31	131.65	127.40
1	AA	807	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	892	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	1070	A	C5-C6-N1	5.30	120.35	117.70
22	BA	1611	C	N1-C2-O2	5.30	122.08	118.90
22	BA	2530	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	2711	A	N3-C4-N9	5.30	131.64	127.40
22	BA	2738	A	N3-C4-N9	5.30	131.64	127.40
55	B8	41	A	N9-C4-C5	5.30	107.92	105.80
1	AA	236	A	N9-C4-C5	5.30	107.92	105.80
1	AA	716	A	N9-C4-C5	5.30	107.92	105.80
22	BA	735	A	C8-N9-C4	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1096	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1134	A	C8-N9-C4	5.30	107.92	105.80
23	BB	108	A	C5-C6-N1	5.30	120.35	117.70
1	AA	1447	A	N9-C4-C5	5.30	107.92	105.80
22	BA	1032	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1359	A	C5-C6-N1	5.30	120.35	117.70
22	BA	2829	A	C4-C5-C6	5.30	119.65	117.00
22	BA	1698	A	C5-C6-N1	5.30	120.35	117.70
1	AA	496	A	N9-C4-C5	5.30	107.92	105.80
22	BA	1134	A	N9-C4-C5	5.30	107.92	105.80
22	BA	2851	A	C8-N9-C4	5.30	107.92	105.80
1	AA	753	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1158	C	C2-N1-C1'	5.29	124.62	118.80
22	BA	217	A	C5-C6-N1	5.29	120.35	117.70
22	BA	1495	A	N3-C4-N9	5.29	131.64	127.40
1	AA	696	A	C8-N9-C4	5.29	107.92	105.80
1	AA	1287	A	N9-C4-C5	5.29	107.92	105.80
22	BA	2823	A	C5-C6-N1	5.29	120.35	117.70
22	BA	2873	A	C5-C6-N1	5.29	120.35	117.70
1	AA	109	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	665	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1251	A	C4-C5-C6	5.29	119.65	117.00
22	BA	155	A	C8-N9-C4	5.29	107.92	105.80
22	BA	1522	A	C4-C5-C6	5.29	119.65	117.00
22	BA	1927	A	C4-C5-C6	5.29	119.65	117.00
22	BA	2266	A	C4-C5-C6	5.29	119.64	117.00
22	BA	2468	A	N3-C4-N9	5.29	131.63	127.40
55	B8	21	A	N9-C4-C5	5.29	107.92	105.80
22	BA	2328	A	C5-C6-N1	5.29	120.34	117.70
22	BA	2392	A	N3-C4-N9	5.29	131.63	127.40
23	BB	66	A	C8-N9-C4	5.29	107.92	105.80
1	AA	3	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	718	A	C5-C6-N1	5.29	120.34	117.70
1	AA	1021	A	C4-C5-C6	5.29	119.64	117.00
1	AA	1531	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1057	A	C4-C5-N7	-5.29	108.06	110.70
55	B8	26	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	262	A	N9-C4-C5	5.29	107.92	105.80
22	BA	1525	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1677	A	N3-C4-N9	5.29	131.63	127.40
1	AA	681	A	N9-C4-C5	5.29	107.91	105.80
22	BA	1494	A	N3-C4-N9	5.29	131.63	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1780	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	1430	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1668	A	N3-C4-N9	5.28	131.63	127.40
22	BA	1912	A	C5-C6-N1	5.28	120.34	117.70
1	AA	1503	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1513	A	C5-C6-N1	5.28	120.34	117.70
22	BA	44	A	C5-C6-N1	5.28	120.34	117.70
22	BA	1757	A	N3-C4-N9	5.28	131.62	127.40
1	AA	630	A	C8-N9-C4	5.28	107.91	105.80
22	BA	320	A	C4-C5-C6	5.28	119.64	117.00
22	BA	2614	A	C5-C6-N1	5.28	120.34	117.70
22	BA	2800	A	C5-C6-N1	5.28	120.34	117.70
22	BA	1302	A	N3-C4-N9	5.28	131.62	127.40
1	AA	162	A	C8-N9-C4	5.28	107.91	105.80
1	AA	959	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	933	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1111	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1395	A	C4-C5-N7	-5.28	108.06	110.70
23	BB	15	A	N3-C4-N9	5.28	131.62	127.40
1	AA	236	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1340	A	C4-C5-C6	5.28	119.64	117.00
1	AA	1398	A	N9-C4-C5	5.28	107.91	105.80
22	BA	501	A	N3-C4-N9	5.28	131.62	127.40
22	BA	1067	A	C5-C6-N1	5.28	120.34	117.70
1	AA	102	G	O4'-C1'-N9	5.27	112.42	108.20
22	BA	219	A	C5-C6-N1	5.27	120.34	117.70
22	BA	1728	C	N1-C2-N3	5.27	122.89	119.20
55	B8	73	A	C8-N9-C4	5.27	107.91	105.80
1	AA	53	A	C8-N9-C4	5.27	107.91	105.80
1	AA	364	A	C8-N9-C4	5.27	107.91	105.80
1	AA	715	A	C5-C6-N1	5.27	120.34	117.70
22	BA	2810	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	2851	A	C5-C6-N1	5.27	120.34	117.70
1	AA	1167	A	N9-C4-C5	5.27	107.91	105.80
22	BA	2764	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	2883	A	C5-C6-N1	5.27	120.34	117.70
1	AA	1256	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	501	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1676	A	N3-C4-N9	5.27	131.62	127.40
1	AA	7	A	N3-C4-N9	5.27	131.61	127.40
1	AA	1105	A	N3-C4-N9	5.27	131.61	127.40
1	AA	1339	A	C5-C6-N1	5.27	120.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	505	A	C4-C5-N7	-5.27	108.07	110.70
22	BA	749	A	C4-C5-C6	5.27	119.63	117.00
22	BA	2071	A	C4-C5-C6	5.27	119.63	117.00
22	BA	2411	A	C5-C6-N1	5.27	120.33	117.70
1	AA	958	A	C4-C5-C6	5.26	119.63	117.00
22	BA	943	A	C6-N1-C2	5.26	121.76	118.60
22	BA	1157	G	C8-N9-C1'	-5.26	120.16	127.00
22	BA	2227	A	C4-C5-C6	5.26	119.63	117.00
22	BA	2835	A	N9-C4-C5	5.26	107.91	105.80
23	BB	46	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	649	A	C5-C6-N1	5.26	120.33	117.70
22	BA	1342	A	N9-C4-C5	5.26	107.91	105.80
22	BA	1900	A	N9-C4-C5	5.26	107.91	105.80
22	BA	2654	A	C8-N9-C4	5.26	107.91	105.80
22	BA	2749	A	N3-C4-N9	5.26	131.61	127.40
22	BA	1151	A	N9-C4-C5	5.26	107.90	105.80
55	B8	38	A	N3-C4-N9	5.26	131.61	127.40
1	AA	412	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	460	A	C5-C6-N1	5.26	120.33	117.70
1	AA	1163	A	C4-C5-C6	5.26	119.63	117.00
1	AA	1430	A	C4-C5-C6	5.26	119.63	117.00
22	BA	74	A	C4-C5-C6	5.26	119.63	117.00
22	BA	1070	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	2406	A	N3-C4-N9	5.26	131.61	127.40
22	BA	2435	A	N9-C4-C5	5.26	107.90	105.80
22	BA	352	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	979	A	N3-C4-N9	5.26	131.61	127.40
22	BA	1701	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	1964	G	O4'-C1'-N9	-5.26	104.00	108.20
22	BA	2183	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2727	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2761	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	637	A	N9-C4-C5	5.25	107.90	105.80
1	AA	560	A	C5-C6-N1	5.25	120.33	117.70
22	BA	6	A	N3-C4-N9	5.25	131.60	127.40
1	AA	327	A	C4-C5-N7	-5.25	108.07	110.70
1	AA	596	A	C5-C6-N1	5.25	120.33	117.70
1	AA	681	A	C4-C5-C6	5.25	119.63	117.00
22	BA	603	A	N3-C4-N9	5.25	131.60	127.40
22	BA	670	A	C5-C6-N1	5.25	120.33	117.70
22	BA	699	A	N3-C4-N9	5.25	131.60	127.40
22	BA	1591	A	C4-C5-N7	-5.25	108.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	182	A	C4-C5-C6	5.25	119.62	117.00
1	AA	1092	A	N9-C4-C5	5.25	107.90	105.80
1	AA	439	U	C2-N3-C4	-5.25	123.85	127.00
1	AA	787	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	227	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	556	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	730	A	C8-N9-C4	5.25	107.90	105.80
22	BA	752	A	C4-C5-C6	5.25	119.62	117.00
22	BA	1570	A	N9-C4-C5	5.25	107.90	105.80
22	BA	586	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	1676	A	C5-N7-C8	5.25	106.52	103.90
22	BA	1819	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	2273	A	C5-C6-N1	5.25	120.32	117.70
1	AA	172	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	1130	A	C8-N9-C4	5.25	107.90	105.80
22	BA	1580	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	1092	A	N3-C4-N9	5.24	131.59	127.40
1	AA	1093	A	C8-N9-C4	5.24	107.90	105.80
1	AA	1346	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	1598	A	C5-C6-N1	5.24	120.32	117.70
22	BA	2191	A	C5-C6-N1	5.24	120.32	117.70
1	AA	694	A	C5-C6-N1	5.24	120.32	117.70
1	AA	845	A	C4-C5-C6	5.24	119.62	117.00
22	BA	1603	A	C8-N9-C4	5.24	107.90	105.80
22	BA	1746	A	C5-C6-N1	5.24	120.32	117.70
1	AA	622	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	309	A	C5-C6-N1	5.24	120.32	117.70
22	BA	472	A	C4-C5-C6	5.24	119.62	117.00
22	BA	918	A	N3-C4-N9	5.24	131.59	127.40
22	BA	1613	G	C4-C5-N7	-5.24	108.70	110.80
22	BA	2163	A	N3-C4-N9	5.24	131.59	127.40
22	BA	146	A	N9-C4-C5	5.24	107.90	105.80
22	BA	917	A	C8-N9-C4	5.24	107.90	105.80
22	BA	1637	A	C4-C5-C6	5.24	119.62	117.00
22	BA	2497	A	O5'-P-OP1	-5.24	100.98	105.70
22	BA	2776	A	C4-C5-C6	5.24	119.62	117.00
23	BB	115	A	N9-C4-C5	5.24	107.90	105.80
22	BA	226	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	344	A	C4-C5-C6	5.24	119.62	117.00
1	AA	313	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	765	C	C6-N1-C2	-5.24	118.21	120.30
22	BA	1858	A	C4-C5-C6	5.24	119.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2322	A	C5-C6-N1	5.24	120.32	117.70
23	BB	99	A	C8-N9-C4	5.24	107.89	105.80
1	AA	33	A	C5-C6-N1	5.23	120.32	117.70
22	BA	574	A	C8-N9-C4	5.23	107.89	105.80
22	BA	2740	A	C8-N9-C4	5.23	107.89	105.80
1	AA	77	A	C4-C5-C6	5.23	119.62	117.00
1	AA	574	A	N9-C4-C5	5.23	107.89	105.80
1	AA	1035	A	C4-C5-C6	5.23	119.62	117.00
22	BA	27	G	O4'-C1'-N9	5.23	112.39	108.20
22	BA	265	A	C4-C5-C6	5.23	119.62	117.00
22	BA	342	A	C4-C5-C6	5.23	119.62	117.00
22	BA	878	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	985	C	N3-C2-O2	-5.23	118.24	121.90
22	BA	2135	A	C5-C6-N1	5.23	120.32	117.70
22	BA	2336	A	C4-C5-C6	5.23	119.62	117.00
22	BA	265	A	C5-C6-N1	5.23	120.31	117.70
22	BA	514	A	N3-C4-N9	5.23	131.59	127.40
22	BA	1098	A	N9-C4-C5	5.23	107.89	105.80
22	BA	1304	A	C5-C6-N1	5.23	120.31	117.70
55	B8	6	A	N3-C4-N9	5.23	131.59	127.40
55	B8	38	A	C4-C5-N7	-5.23	108.08	110.70
1	AA	196	A	C5-C6-N1	5.23	120.31	117.70
22	BA	422	A	C8-N9-C4	5.23	107.89	105.80
22	BA	1304	A	C4-C5-N7	-5.23	108.09	110.70
1	AA	676	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	728	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1437	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	1794	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	321	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	878	A	C5-C6-N1	5.22	120.31	117.70
22	BA	1937	A	C8-N9-C4	5.22	107.89	105.80
22	BA	2577	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	816	A	C4-C5-C6	5.22	119.61	117.00
1	AA	431	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	74	A	N9-C4-C5	5.22	107.89	105.80
22	BA	165	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	322	A	C8-N9-C4	5.22	107.89	105.80
22	BA	512	G	N3-C4-N9	-5.22	122.87	126.00
22	BA	1322	A	C4-C5-C6	5.22	119.61	117.00
22	BA	2645	G	O4'-C1'-N9	5.22	112.38	108.20
22	BA	2719	G	C8-N9-C4	5.22	108.49	106.40
22	BA	592	A	C5-C6-N1	5.22	120.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1032	A	N9-C4-C5	5.22	107.89	105.80
1	AA	120	A	C5-C6-N1	5.22	120.31	117.70
1	AA	909	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	695	A	C5-C6-N1	5.21	120.31	117.70
1	AA	728	A	C8-N9-C4	5.21	107.89	105.80
1	AA	1152	A	C8-N9-C4	5.21	107.89	105.80
22	BA	233	A	C4-C5-C6	5.21	119.61	117.00
22	BA	2448	A	C5-C6-N1	5.21	120.31	117.70
22	BA	1663	G	OP1-P-O3'	5.21	116.67	105.20
1	AA	262	A	C5-C6-N1	5.21	120.31	117.70
1	AA	363	A	N9-C4-C5	5.21	107.89	105.80
1	AA	978	A	N3-C4-N9	5.21	131.57	127.40
1	AA	1271	A	C5-C6-N1	5.21	120.31	117.70
22	BA	1439	A	C8-N9-C4	5.21	107.88	105.80
22	BA	2778	A	C5-C6-N1	5.21	120.31	117.70
1	AA	253	A	N9-C4-C5	5.21	107.88	105.80
1	AA	766	A	C5-C6-N1	5.21	120.31	117.70
1	AA	1261	A	C8-N9-C4	5.21	107.88	105.80
22	BA	1276	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	2309	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	1556	C	N3-C4-N4	-5.21	114.36	118.00
22	BA	2476	A	C4-C5-C6	5.21	119.60	117.00
1	AA	195	A	N9-C4-C5	5.21	107.88	105.80
1	AA	270	A	C8-N9-C4	5.21	107.88	105.80
1	AA	1508	A	C8-N9-C4	5.21	107.88	105.80
22	BA	95	A	N9-C4-C5	5.21	107.88	105.80
22	BA	941	A	C5-C6-N1	5.21	120.30	117.70
22	BA	1265	A	C4-C5-C6	5.21	119.60	117.00
22	BA	1001	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1226	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1583	A	C4-C5-C6	5.20	119.60	117.00
22	BA	727	A	C5-C6-N1	5.20	120.30	117.70
22	BA	2478	A	C5-C6-N1	5.20	120.30	117.70
23	BB	59	A	C6-N1-C2	-5.20	115.48	118.60
1	AA	28	A	N9-C4-C5	5.20	107.88	105.80
1	AA	431	A	N3-C4-N9	5.20	131.56	127.40
1	AA	1465	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	402	A	C8-N9-C4	5.20	107.88	105.80
22	BA	572	A	C5-C6-N1	5.20	120.30	117.70
22	BA	621	A	N3-C4-N9	5.20	131.56	127.40
22	BA	1312	U	C6-N1-C1'	5.20	128.48	121.20
1	AA	1288	A	C4-C5-N7	-5.20	108.10	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	183	C	C6-N1-C2	-5.20	118.22	120.30
22	BA	586	A	N9-C4-C5	5.20	107.88	105.80
23	BB	99	A	N3-C4-N9	5.20	131.56	127.40
55	B8	59	A	C8-N9-C4	5.20	107.88	105.80
1	AA	1110	A	N9-C4-C5	5.20	107.88	105.80
22	BA	53	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	196	A	C5-C6-N1	5.20	120.30	117.70
1	AA	533	A	N9-C4-C5	5.20	107.88	105.80
22	BA	644	A	C5-C6-N1	5.20	120.30	117.70
1	AA	1004	A	N9-C4-C5	5.19	107.88	105.80
22	BA	613	A	C4-C5-C6	5.19	119.60	117.00
1	AA	320	A	C4-C5-C6	5.19	119.60	117.00
1	AA	648	A	C4-C5-C6	5.19	119.60	117.00
1	AA	825	A	C4-C5-C6	5.19	119.60	117.00
1	AA	977	A	C8-N9-C4	5.19	107.88	105.80
22	BA	244	A	C4-C5-N7	-5.19	108.10	110.70
22	BA	1596	A	C5-C6-N1	5.19	120.30	117.70
22	BA	2882	A	C4-C5-C6	5.19	119.60	117.00
22	BA	2003	A	C8-N9-C4	5.19	107.88	105.80
22	BA	2639	A	C8-N9-C4	5.19	107.88	105.80
23	BB	78	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	968	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1495	A	N9-C4-C5	5.19	107.88	105.80
22	BA	1509	A	N9-C4-C5	5.19	107.88	105.80
22	BA	2358	A	C4-C5-C6	5.19	119.59	117.00
1	AA	155	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	493	A	C4-C5-C6	5.19	119.59	117.00
1	AA	1306	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	423	A	C8-N9-C4	5.19	107.88	105.80
1	AA	139	A	C8-N9-C4	5.18	107.87	105.80
22	BA	103	A	C5-C6-N1	5.18	120.29	117.70
22	BA	670	A	C4-C5-C6	5.18	119.59	117.00
22	BA	972	A	C4-C5-C6	5.18	119.59	117.00
22	BA	2072	C	C6-N1-C2	-5.18	118.23	120.30
1	AA	1145	A	C8-N9-C4	5.18	107.87	105.80
22	BA	278	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	89	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	809	G	N1-C6-O6	-5.18	116.79	119.90
22	BA	2340	A	C4-C5-C6	5.18	119.59	117.00
1	AA	160	A	N3-C4-N9	5.18	131.54	127.40
1	AA	250	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	2278	A	N3-C4-N9	5.18	131.54	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	819	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	1155	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	892	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1147	A	N3-C4-N9	5.18	131.54	127.40
22	BA	1453	A	N9-C4-C5	5.18	107.87	105.80
22	BA	1970	A	C4-C5-C6	5.18	119.59	117.00
22	BA	2170	A	C5-C6-N1	5.18	120.29	117.70
55	B8	14	A	C5-C6-N1	5.18	120.29	117.70
1	AA	509	A	N9-C4-C5	5.17	107.87	105.80
1	AA	759	A	C4-C5-C6	5.17	119.59	117.00
22	BA	1598	A	C4-C5-C6	5.17	119.59	117.00
22	BA	2191	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	2225	A	N3-C4-N9	5.17	131.54	127.40
23	BB	34	A	C4-C5-C6	5.17	119.59	117.00
1	AA	1271	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1280	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	354	A	C5-C6-N1	5.17	120.29	117.70
1	AA	16	A	N9-C4-C5	5.17	107.87	105.80
1	AA	274	A	N9-C4-C5	5.17	107.87	105.80
1	AA	864	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	1952	A	C5-C6-N1	5.17	120.29	117.70
22	BA	2882	A	N3-C4-N9	5.17	131.54	127.40
22	BA	555	G	C8-N9-C1'	-5.17	120.28	127.00
22	BA	1025	G	C8-N9-C4	-5.17	104.33	106.40
22	BA	1690	A	N3-C4-N9	5.17	131.54	127.40
23	BB	115	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2014	A	N9-C4-C5	5.17	107.87	105.80
22	BA	2025	C	C6-N1-C2	-5.17	118.23	120.30
22	BA	2531	A	C5-C6-N1	5.17	120.28	117.70
22	BA	282	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	928	A	C8-N9-C4	5.17	107.87	105.80
1	AA	831	A	C4-C5-N7	-5.17	108.12	110.70
1	AA	1101	A	N9-C4-C5	5.17	107.87	105.80
22	BA	1913	A	N9-C4-C5	5.17	107.87	105.80
22	BA	2592	G	C6-C5-N7	-5.17	127.30	130.40
22	BA	2700	A	N9-C4-C5	5.17	107.87	105.80
1	AA	26	A	C5-C6-N1	5.16	120.28	117.70
1	AA	189	A	C8-N9-C4	5.16	107.87	105.80
1	AA	451	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	923	A	C5-C6-N1	5.16	120.28	117.70
1	AA	1019	A	C5-C6-N1	5.16	120.28	117.70
22	BA	218	A	C5-C6-N1	5.16	120.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	590	A	N3-C4-N9	5.16	131.53	127.40
22	BA	1322	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1785	A	C5-C6-N1	5.16	120.28	117.70
55	B8	58	A	N9-C4-C5	5.16	107.87	105.80
1	AA	171	A	N3-C4-N9	5.16	131.53	127.40
1	AA	1022	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1239	A	C4-C5-C6	5.16	119.58	117.00
1	AA	1394	A	N9-C4-C5	5.16	107.86	105.80
22	BA	348	A	C5-C6-N1	5.16	120.28	117.70
22	BA	362	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	504	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2134	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	2478	A	N9-C4-C5	5.16	107.86	105.80
1	AA	459	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	1016	A	C4-C5-C6	5.16	119.58	117.00
22	BA	352	A	C5-C6-N1	5.16	120.28	117.70
22	BA	1084	A	N3-C4-N9	5.16	131.53	127.40
22	BA	2753	A	C4-C5-C6	5.16	119.58	117.00
22	BA	1586	A	N3-C4-N9	5.16	131.53	127.40
22	BA	2352	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	2	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	363	A	C5-C6-N1	5.16	120.28	117.70
1	AA	1534	A	C8-N9-C4	5.16	107.86	105.80
23	BB	57	A	C8-N9-C4	5.16	107.86	105.80
1	AA	8	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	2274	A	N9-C4-C5	5.15	107.86	105.80
1	AA	53	A	N9-C4-C5	5.15	107.86	105.80
22	BA	1353	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	1918	A	N3-C4-N9	5.15	131.52	127.40
23	BB	73	A	C4-C5-C6	5.15	119.58	117.00
1	AA	482	A	C5-C6-N1	5.15	120.28	117.70
1	AA	493	A	N3-C4-N9	5.15	131.52	127.40
1	AA	1374	A	N9-C4-C5	5.15	107.86	105.80
22	BA	439	A	C8-N9-C4	5.15	107.86	105.80
22	BA	1535	A	C4-C5-C6	5.15	119.57	117.00
22	BA	943	A	C8-N9-C4	5.15	107.86	105.80
22	BA	1365	A	C8-N9-C4	5.15	107.86	105.80
22	BA	1545	A	C4-C5-C6	5.15	119.57	117.00
1	AA	1239	A	N3-C4-N9	5.15	131.52	127.40
1	AA	1311	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	965	C	OP2-P-O3'	5.15	116.52	105.20
22	BA	2406	A	N9-C4-C5	5.14	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2846	G	N1-C6-O6	-5.14	116.81	119.90
1	AA	635	A	C5-C6-N1	5.14	120.27	117.70
1	AA	1105	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1398	A	C4-C5-C6	5.14	119.57	117.00
22	BA	430	A	N9-C4-C5	5.14	107.86	105.80
22	BA	1312	U	C2-N1-C1'	-5.14	111.53	117.70
22	BA	1614	A	N3-C4-N9	5.14	131.51	127.40
1	AA	8	A	N9-C4-C5	5.14	107.86	105.80
22	BA	1711	A	C4-C5-C6	5.14	119.57	117.00
1	AA	938	A	C5-C6-N1	5.14	120.27	117.70
1	AA	1012	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1155	A	N9-C4-C5	5.14	107.86	105.80
22	BA	918	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1641	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1744	A	C5-C6-N1	5.14	120.27	117.70
22	BA	1938	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1993	U	N3-C2-O2	-5.14	118.60	122.20
22	BA	2158	A	C5-C6-N1	5.14	120.27	117.70
22	BA	2741	A	C8-N9-C4	5.14	107.86	105.80
22	BA	752	A	C5-C6-N1	5.14	120.27	117.70
1	AA	1428	A	C8-N9-C4	5.14	107.86	105.80
22	BA	126	A	N3-C4-N9	5.14	131.51	127.40
22	BA	1253	A	C5-N7-C8	5.14	106.47	103.90
22	BA	2426	A	C4-C5-C6	5.14	119.57	117.00
22	BA	575	A	N3-C4-N9	5.13	131.51	127.40
22	BA	1077	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2270	A	N9-C4-C5	5.13	107.85	105.80
22	BA	2469	A	C4-C5-C6	5.13	119.57	117.00
55	B8	6	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2199	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2592	G	C4-N9-C1'	5.13	133.17	126.50
1	AA	366	A	C8-N9-C4	5.13	107.85	105.80
1	AA	502	A	N9-C4-C5	5.13	107.85	105.80
1	AA	816	A	C5-C6-N1	5.13	120.27	117.70
1	AA	1022	A	N3-C4-N9	5.13	131.50	127.40
22	BA	936	A	N9-C4-C5	5.13	107.85	105.80
22	BA	1286	A	C5-C6-N1	5.13	120.27	117.70
1	AA	583	A	N3-C4-N9	5.13	131.50	127.40
22	BA	382	A	N9-C4-C5	5.13	107.85	105.80
22	BA	761	A	N9-C4-C5	5.13	107.85	105.80
1	AA	3	A	C5-C6-N1	5.13	120.26	117.70
1	AA	120	A	C4-C5-C6	5.13	119.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	143	A	C5-C6-N1	5.13	120.26	117.70
1	AA	509	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	532	A	N9-C4-C5	5.13	107.85	105.80
1	AA	1363	A	C5-C6-N1	5.13	120.26	117.70
22	BA	1640	A	C4-C5-C6	5.13	119.56	117.00
55	B8	66	A	N9-C4-C5	5.13	107.85	105.80
22	BA	2014	A	C8-N9-C4	5.12	107.85	105.80
22	BA	2810	A	N3-C4-N9	5.12	131.50	127.40
23	BB	78	A	C4-C5-C6	5.12	119.56	117.00
1	AA	559	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	1167	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	227	A	C5-C6-N1	5.12	120.26	117.70
22	BA	742	A	C8-N9-C4	5.12	107.85	105.80
22	BA	979	A	C4-C5-C6	5.12	119.56	117.00
22	BA	1241	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1301	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1784	A	C4-C5-C6	5.12	119.56	117.00
22	BA	2019	A	N3-C4-N9	5.12	131.50	127.40
1	AA	143	A	N3-C4-N9	5.12	131.50	127.40
1	AA	977	A	N9-C4-C5	5.12	107.85	105.80
1	AA	1437	A	C5-C6-N1	5.12	120.26	117.70
22	BA	320	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1378	A	N3-C4-N9	5.12	131.50	127.40
22	BA	2810	A	N9-C4-C5	5.12	107.85	105.80
55	B8	58	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1308	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1505	A	C5-C6-N1	5.12	120.26	117.70
1	AA	1158	C	N3-C2-O2	-5.12	118.32	121.90
22	BA	820	A	C8-N9-C4	5.12	107.85	105.80
22	BA	2369	A	C8-N9-C4	5.12	107.85	105.80
22	BA	2814	A	C5-C6-N1	5.12	120.26	117.70
22	BA	532	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1205	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1307	A	C8-N9-C4	5.12	107.85	105.80
1	AA	263	A	C5-C6-N1	5.12	120.26	117.70
1	AA	451	A	C8-N9-C4	5.12	107.85	105.80
1	AA	1446	A	C8-N9-C4	5.12	107.85	105.80
22	BA	216	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	508	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1080	A	C5-C6-N1	5.12	120.26	117.70
22	BA	2324	U	N3-C2-O2	-5.12	118.62	122.20
55	B8	2	G	P-O3'-C3'	5.12	125.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	777	A	C5-C6-N1	5.11	120.26	117.70
22	BA	582	A	C8-N9-C4	5.11	107.84	105.80
22	BA	1626	A	C4-C5-C6	5.11	119.56	117.00
22	BA	1641	A	C4-C5-C6	5.11	119.56	117.00
1	AA	1111	A	C8-N9-C4	5.11	107.84	105.80
22	BA	2776	A	N9-C4-C5	5.11	107.84	105.80
1	AA	50	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	393	A	C4-C5-C6	5.11	119.56	117.00
1	AA	393	A	C5-C6-N1	5.11	120.25	117.70
1	AA	459	A	N9-C4-C5	5.11	107.84	105.80
1	AA	461	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	681	A	N3-C4-N9	5.11	131.49	127.40
1	AA	1437	A	C8-N9-C4	5.11	107.84	105.80
22	BA	2418	A	C4-C5-N7	-5.11	108.14	110.70
22	BA	2778	A	C8-N9-C4	5.11	107.84	105.80
1	AA	938	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1534	A	N9-C4-C5	5.11	107.84	105.80
22	BA	282	A	N9-C4-C5	5.11	107.84	105.80
22	BA	1111	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1938	A	C5-C6-N1	5.11	120.25	117.70
1	AA	139	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	579	A	C5-C6-N1	5.11	120.25	117.70
1	AA	1363	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1205	A	N9-C4-C5	5.11	107.84	105.80
1	AA	784	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	918	A	C5-C6-N1	5.11	120.25	117.70
1	AA	1339	A	C8-N9-C4	5.11	107.84	105.80
22	BA	203	A	N3-C4-N9	5.11	131.49	127.40
22	BA	1378	A	C5-C6-N1	5.11	120.25	117.70
22	BA	1583	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1877	A	C5-C6-N1	5.11	120.25	117.70
22	BA	2592	G	N3-C4-N9	5.11	129.06	126.00
1	AA	129	A	C5-C6-N1	5.10	120.25	117.70
1	AA	325	A	C5-C6-N1	5.10	120.25	117.70
22	BA	73	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	590	A	C5-C6-N1	5.10	120.25	117.70
22	BA	1254	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1522	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2634	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	833	A	C5-C6-N1	5.10	120.25	117.70
22	BA	1504	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2061	G	N3-C4-C5	-5.10	126.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2478	A	N3-C4-N9	5.10	131.48	127.40
1	AA	196	A	N9-C4-C5	5.10	107.84	105.80
1	AA	1238	A	C8-N9-C4	5.10	107.84	105.80
22	BA	471	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	909	A	C4-C5-C6	5.10	119.55	117.00
22	BA	2851	A	N9-C4-C5	5.10	107.84	105.80
1	AA	1493	A	C5-C6-N1	5.10	120.25	117.70
22	BA	627	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2434	A	N9-C4-C5	5.10	107.84	105.80
23	BB	52	A	N3-C4-N9	5.10	131.48	127.40
1	AA	282	A	C4-C5-C6	5.10	119.55	117.00
1	AA	729	A	N3-C4-N9	5.10	131.48	127.40
1	AA	1082	A	C5-C6-N1	5.10	120.25	117.70
1	AA	365	U	N1-C2-O2	5.09	126.37	122.80
1	AA	702	A	C5-C6-N1	5.09	120.25	117.70
1	AA	1225	A	C8-N9-C4	5.09	107.84	105.80
22	BA	460	A	C8-N9-C4	5.09	107.84	105.80
22	BA	626	A	C4-C5-C6	5.09	119.55	117.00
22	BA	2639	A	C4-C5-C6	5.09	119.55	117.00
22	BA	2734	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2880	C	C6-N1-C2	-5.09	118.26	120.30
1	AA	780	A	C5-C6-N1	5.09	120.25	117.70
22	BA	1998	A	C5-C6-N1	5.09	120.25	117.70
1	AA	440	C	N3-C2-O2	-5.09	118.34	121.90
1	AA	1306	A	C5-C6-N1	5.09	120.25	117.70
1	AA	706	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	1717	A	N9-C4-C5	5.09	107.84	105.80
22	BA	2893	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	735	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	2478	A	C8-N9-C4	5.09	107.83	105.80
22	BA	2758	A	C5-C6-N1	5.09	120.24	117.70
22	BA	2813	A	N9-C4-C5	5.09	107.83	105.80
1	AA	1080	A	C8-N9-C4	5.09	107.83	105.80
1	AA	1248	A	N3-C4-N9	5.09	131.47	127.40
22	BA	685	A	C5-C6-N1	5.09	120.24	117.70
22	BA	917	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	1453	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	2453	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	439	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	149	A	C8-N9-C4	5.08	107.83	105.80
1	AA	749	A	C5-C6-N1	5.08	120.24	117.70
1	AA	1360	A	C5-C6-N1	5.08	120.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	226	A	C5-C6-N1	5.08	120.24	117.70
22	BA	1261	C	N3-C4-C5	5.08	123.93	121.90
22	BA	1987	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	2003	A	C5-C6-N1	5.08	120.24	117.70
22	BA	2031	A	N9-C4-C5	5.08	107.83	105.80
22	BA	2542	A	C4-C5-C6	5.08	119.54	117.00
1	AA	151	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	1093	A	N9-C4-C5	5.08	107.83	105.80
22	BA	947	A	C5-C6-N1	5.08	120.24	117.70
22	BA	1285	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1889	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	181	A	C5-C6-N1	5.08	120.24	117.70
1	AA	223	A	N9-C4-C5	5.08	107.83	105.80
1	AA	1251	A	N3-C4-N9	5.08	131.46	127.40
22	BA	492	A	C8-N9-C4	5.08	107.83	105.80
1	AA	560	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	1067	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	65	A	C5-C6-N1	5.07	120.24	117.70
22	BA	1046	A	C5-C6-N1	5.07	120.24	117.70
22	BA	1966	A	N3-C4-N9	5.07	131.46	127.40
22	BA	2378	A	C8-N9-C4	5.07	107.83	105.80
23	BB	15	A	C4-C5-C6	5.07	119.54	117.00
22	BA	1927	A	C4-C5-N7	-5.07	108.16	110.70
55	B8	59	A	N9-C4-C5	5.07	107.83	105.80
1	AA	815	A	N9-C4-C5	5.07	107.83	105.80
1	AA	1022	A	C5-C6-N1	5.07	120.23	117.70
22	BA	340	A	N9-C4-C5	5.07	107.83	105.80
22	BA	368	A	C5-C6-N1	5.07	120.23	117.70
22	BA	391	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1157	G	N3-C4-N9	5.07	129.04	126.00
22	BA	1262	A	C8-N9-C4	5.07	107.83	105.80
22	BA	2700	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	2241	A	N9-C4-C5	5.07	107.83	105.80
22	BA	2518	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1353	A	C8-N9-C4	5.07	107.83	105.80
22	BA	1791	A	N9-C4-C5	5.07	107.83	105.80
1	AA	949	A	C5-C6-N1	5.07	120.23	117.70
22	BA	563	A	N9-C4-C5	5.07	107.83	105.80
22	BA	753	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1901	A	C5-C6-N1	5.07	120.23	117.70
22	BA	1912	A	C8-N9-C4	5.07	107.83	105.80
22	BA	2184	A	C8-N9-C4	5.07	107.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2810	A	C4-C5-C6	5.07	119.53	117.00
22	BA	371	A	N3-C4-N9	5.06	131.45	127.40
22	BA	1679	A	C5-C6-N1	5.06	120.23	117.70
22	BA	466	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1505	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	2328	A	N9-C4-C5	5.06	107.83	105.80
1	AA	461	A	C8-N9-C4	5.06	107.82	105.80
22	BA	616	A	N9-C4-C5	5.06	107.82	105.80
22	BA	878	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1285	A	C8-N9-C4	5.06	107.82	105.80
22	BA	1496	A	C8-N9-C4	5.06	107.83	105.80
22	BA	1503	A	C8-N9-C4	5.06	107.82	105.80
1	AA	238	A	N3-C4-N9	5.06	131.45	127.40
22	BA	1385	A	N3-C4-N9	5.06	131.45	127.40
22	BA	1528	A	C5-C6-N1	5.06	120.23	117.70
22	BA	2035	G	N1-C6-O6	-5.06	116.86	119.90
22	BA	2750	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1311	G	N7-C8-N9	5.06	115.63	113.10
22	BA	586	A	N3-C4-N9	5.05	131.44	127.40
22	BA	1010	A	N3-C4-N9	5.05	131.44	127.40
22	BA	1028	A	C4-C5-C6	5.05	119.53	117.00
22	BA	1783	A	N9-C4-C5	5.05	107.82	105.80
22	BA	2381	A	N3-C4-N9	5.05	131.44	127.40
1	AA	279	A	N9-C4-C5	5.05	107.82	105.80
1	AA	996	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	1019	A	N9-C4-C5	5.05	107.82	105.80
22	BA	1098	A	C5-C6-N1	5.05	120.23	117.70
55	B8	42	A	C8-N9-C4	5.05	107.82	105.80
1	AA	602	A	N9-C4-C5	5.05	107.82	105.80
22	BA	73	A	C8-N9-C4	5.05	107.82	105.80
1	AA	1021	A	C5-C6-N1	5.05	120.22	117.70
22	BA	492	A	N9-C4-C5	5.05	107.82	105.80
22	BA	541	A	C5-C6-N1	5.05	120.22	117.70
22	BA	1194	A	N9-C4-C5	5.05	107.82	105.80
1	AA	958	A	N3-C4-N9	5.05	131.44	127.40
1	AA	1044	A	C5-C6-N1	5.05	120.22	117.70
22	BA	2282	G	C5-C6-O6	5.05	131.63	128.60
23	BB	104	A	N9-C4-C5	5.05	107.82	105.80
1	AA	629	A	N9-C4-C5	5.05	107.82	105.80
1	AA	1318	A	C5-C6-N1	5.05	120.22	117.70
1	AA	1531	A	C8-N9-C4	5.05	107.82	105.80
22	BA	149	A	N9-C4-C5	5.05	107.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2095	A	N9-C4-C5	5.05	107.82	105.80
22	BA	2434	A	C4-C5-N7	-5.05	108.18	110.70
1	AA	65	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	892	A	N9-C4-C5	5.04	107.82	105.80
1	AA	923	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	1012	A	C8-N9-C4	5.04	107.82	105.80
22	BA	1000	A	C8-N9-C4	5.04	107.82	105.80
22	BA	1616	A	C5-N7-C8	5.04	106.42	103.90
22	BA	2135	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2531	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	831	A	C5-C6-N1	5.04	120.22	117.70
22	BA	73	A	N3-C4-N9	5.04	131.43	127.40
22	BA	1632	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	1641	A	N3-C4-N9	5.04	131.43	127.40
22	BA	2010	G	N1-C6-O6	-5.04	116.88	119.90
23	BB	50	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	414	A	C5-C6-N1	5.04	120.22	117.70
1	AA	602	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	785	G	O5'-P-OP2	-5.04	101.16	105.70
22	BA	149	A	C5-C6-N1	5.04	120.22	117.70
22	BA	655	A	N9-C4-C5	5.04	107.82	105.80
22	BA	802	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2572	A	N3-C4-N9	5.04	131.43	127.40
1	AA	559	A	C5-C6-N1	5.04	120.22	117.70
1	AA	1441	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	689	A	C4-C5-C6	5.04	119.52	117.00
1	AA	274	A	C5-C6-N1	5.04	120.22	117.70
1	AA	465	A	C8-N9-C4	5.04	107.81	105.80
1	AA	532	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	125	A	N9-C4-C5	5.04	107.81	105.80
22	BA	693	A	N9-C4-C5	5.04	107.81	105.80
22	BA	804	A	C4-C5-C6	5.04	119.52	117.00
22	BA	1226	A	C8-N9-C4	5.04	107.81	105.80
22	BA	2813	A	C8-N9-C4	5.04	107.81	105.80
1	AA	274	A	C4-C5-C6	5.03	119.52	117.00
1	AA	889	A	C4-C5-C6	5.03	119.52	117.00
1	AA	974	A	C5-C6-N1	5.03	120.22	117.70
1	AA	1145	A	C4-C5-C6	5.03	119.52	117.00
1	AA	1274	A	N9-C4-C5	5.03	107.81	105.80
22	BA	668	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	1342	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	1885	A	C5-C6-N1	5.03	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	348	A	N3-C4-N9	5.03	131.43	127.40
22	BA	497	A	C4-C5-C6	5.03	119.52	117.00
22	BA	782	A	C4-C5-N7	-5.03	108.18	110.70
1	AA	560	A	C8-N9-C4	5.03	107.81	105.80
22	BA	1264	A	C4-C5-C6	5.03	119.52	117.00
22	BA	1877	A	C8-N9-C4	5.03	107.81	105.80
22	BA	2679	A	C8-N9-C4	5.03	107.81	105.80
23	BB	115	A	N3-C4-N9	5.03	131.42	127.40
55	B8	66	A	C5-C6-N1	5.03	120.22	117.70
1	AA	560	A	N9-C4-C5	5.03	107.81	105.80
1	AA	649	A	N9-C4-C5	5.03	107.81	105.80
22	BA	348	A	C4-C5-C6	5.03	119.51	117.00
22	BA	616	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1204	A	C5-C6-N1	5.03	120.21	117.70
22	BA	2169	A	C8-N9-C4	5.03	107.81	105.80
1	AA	8	A	C4-C5-C6	5.03	119.51	117.00
1	AA	630	A	N9-C4-C5	5.03	107.81	105.80
22	BA	204	A	C4-C5-C6	5.03	119.51	117.00
22	BA	1420	A	C4-C5-C6	5.03	119.51	117.00
55	B8	38	A	C5-C6-N1	5.03	120.21	117.70
1	AA	892	A	C5-C6-N1	5.03	120.21	117.70
1	AA	574	A	C5-C6-N1	5.02	120.21	117.70
1	AA	1196	A	N3-C4-N9	5.02	131.42	127.40
22	BA	1327	A	C4-C5-C6	5.02	119.51	117.00
22	BA	1853	A	N3-C4-N9	5.02	131.42	127.40
1	AA	223	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	233	A	C5-C6-N1	5.02	120.21	117.70
1	AA	253	A	C5-C6-N1	5.02	120.21	117.70
1	AA	1036	A	N3-C4-N9	5.02	131.42	127.40
1	AA	1110	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	2171	A	C4-C5-N7	-5.02	108.19	110.70
1	AA	16	A	N3-C4-N9	5.02	131.41	127.40
1	AA	465	A	C4-C5-N7	-5.02	108.19	110.70
1	AA	675	A	N3-C4-N9	5.02	131.41	127.40
22	BA	1067	A	N9-C4-C5	5.02	107.81	105.80
22	BA	1930	G	C4-N9-C1'	-5.02	119.98	126.50
22	BA	2212	A	C5-C6-N1	5.02	120.21	117.70
1	AA	243	A	C4-C5-C6	5.02	119.51	117.00
1	AA	1362	A	N9-C4-C5	5.02	107.81	105.80
1	AA	1413	A	C5-C6-N1	5.02	120.21	117.70
22	BA	460	A	N9-C4-C5	5.02	107.81	105.80
22	BA	892	A	N9-C4-C5	5.02	107.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2033	A	C4-C5-C6	5.02	119.51	117.00
1	AA	1248	A	C8-N9-C4	5.02	107.81	105.80
1	AA	1285	A	N3-C4-N9	5.02	131.41	127.40
22	BA	2753	A	N3-C4-N9	5.02	131.41	127.40
55	B8	58	A	C4-C5-N7	-5.02	108.19	110.70
1	AA	906	A	C5-C6-N1	5.01	120.21	117.70
1	AA	1465	A	N9-C4-C5	5.01	107.81	105.80
22	BA	127	A	N3-C4-N9	5.01	131.41	127.40
22	BA	905	A	N9-C4-C5	5.01	107.81	105.80
22	BA	1632	A	N9-C4-C5	5.01	107.81	105.80
22	BA	1821	A	C4-C5-C6	5.01	119.51	117.00
22	BA	2634	A	N9-C4-C5	5.01	107.81	105.80
1	AA	676	A	C5-C6-N1	5.01	120.21	117.70
22	BA	233	A	N3-C4-N9	5.01	131.41	127.40
22	BA	1194	A	N3-C4-N9	5.01	131.41	127.40
22	BA	1385	A	N9-C4-C5	5.01	107.81	105.80
22	BA	2392	A	C5-C6-N1	5.01	120.20	117.70
22	BA	2476	A	N3-C4-N9	5.01	131.41	127.40
1	AA	303	A	C5-C6-N1	5.01	120.20	117.70
1	AA	1014	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	1014	A	N9-C4-C5	5.01	107.80	105.80
1	AA	95	C	N1-C2-O2	5.01	121.91	118.90
22	BA	2205	A	C8-N9-C4	5.01	107.80	105.80
1	AA	696	A	C4-C5-N7	-5.01	108.20	110.70
1	AA	1368	A	C4-C5-N7	-5.01	108.20	110.70
22	BA	345	A	C5-C6-N1	5.01	120.20	117.70
22	BA	564	C	N3-C2-O2	-5.01	118.40	121.90
1	AA	119	A	N9-C4-C5	5.00	107.80	105.80
1	AA	448	A	C8-N9-C4	5.00	107.80	105.80
1	AA	101	A	C8-N9-C4	5.00	107.80	105.80
1	AA	195	A	C4-C5-C6	5.00	119.50	117.00
22	BA	1264	A	C5-C6-N1	5.00	120.20	117.70
22	BA	2736	A	C5-C6-N1	5.00	120.20	117.70
1	AA	816	A	N9-C4-C5	5.00	107.80	105.80
1	AA	1022	A	C4-C5-N7	-5.00	108.20	110.70
1	AA	1311	A	C8-N9-C4	5.00	107.80	105.80
22	BA	1701	A	N3-C4-N9	5.00	131.40	127.40
22	BA	1847	A	C8-N9-C4	5.00	107.80	105.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16583	454	0
2	AB	1753	0	1780	34	0
3	AC	1624	0	1696	33	0
4	AD	1643	0	1707	20	0
5	AE	1144	0	1185	18	0
6	AF	862	0	864	21	0
7	AG	1181	0	1238	28	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	39	0
10	AJ	795	0	836	25	0
11	AK	877	0	887	19	0
12	AL	957	0	1017	19	0
13	AM	883	0	941	28	0
14	AN	799	0	841	23	0
15	AO	714	0	734	2	0
16	AP	649	0	666	9	0
17	AQ	648	0	691	10	0
18	AR	455	0	478	10	0
19	AS	656	0	680	24	0
20	AT	670	0	719	7	0
21	AU	465	0	491	11	0
22	BA	62209	0	31287	446	0
23	BB	2569	0	1301	19	0
24	BC	2082	0	2154	26	0
25	BD	1566	0	1618	18	0
26	BE	1552	0	1619	18	0
27	BF	1410	0	1444	38	0
28	BG	1323	0	1371	14	0
29	BH	1110	0	1148	31	0
30	BI	522	0	520	23	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BL	1053	0	1128	15	0
34	BM	1075	0	1155	13	0
35	BN	945	0	989	7	0
36	BO	900	0	935	7	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	11	0
39	BR	816	0	839	7	0
40	BS	857	0	922	12	0
41	BT	738	0	807	17	0
42	BU	779	0	831	18	0
43	BV	753	0	780	10	0
44	BW	580	0	594	11	0
45	BX	625	0	652	2	0
46	BY	501	0	531	4	0
47	BZ	449	0	488	8	0
48	B0	444	0	458	7	0
49	B1	414	0	442	6	0
50	B2	377	0	418	3	0
51	B3	504	0	572	16	0
52	B4	302	0	340	3	0
53	B5	146	0	139	5	0
54	B7	211	0	110	5	0
55	B8	1646	0	831	26	0
56	B9	2768	0	2666	86	0
57	AA	87	0	0	0	0
57	B8	2	0	0	0	0
57	BA	243	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	2	0	0	0	0
57	BL	3	0	0	0	0
58	AA	38	0	0	0	0
58	AM	1	0	0	0	0
58	BA	104	0	0	0	0
58	BB	1	0	0	0	0
58	BC	1	0	0	0	0
58	BD	1	0	0	0	0
58	BM	1	0	0	0	0
59	AB	1	0	0	0	0
59	B4	1	0	0	0	0
59	BI	1	0	0	0	0
60	BA	15	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AA	167	0	0	0	0
61	AK	1	0	0	0	0
61	AM	1	0	0	0	0
61	AN	3	0	0	0	0
61	BA	617	0	0	3	0
61	BC	6	0	0	0	0
61	BD	2	0	0	0	0
61	BN	3	0	0	0	0
All	All	148175	0	99399	1626	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B8:1:C:H5'	56:B9:282:LYS:NZ	1.70	1.05
22:BA:2185:U:C4	22:BA:2186:G:O6	2.13	1.00
1:AA:1088:G:N2	1:AA:1167:A:H61	1.59	1.00
1:AA:1026:G:C6	1:AA:1035:A:N6	2.32	0.98
22:BA:884:U:O4	22:BA:892:A:C5	2.21	0.93
1:AA:1088:G:H21	1:AA:1167:A:H61	0.96	0.92
1:AA:445:G:H1	1:AA:489:C:H5	1.20	0.90
1:AA:100:G:H4'	1:AA:101:A:O5'	1.71	0.89
22:BA:2107:G:H1	22:BA:2182:U:H3	1.17	0.89
1:AA:1026:G:N1	1:AA:1035:A:C6	2.41	0.89
8:AH:12:THR:HG22	8:AH:15:ARG:HH12	1.37	0.89
1:AA:1026:G:C6	1:AA:1035:A:C6	2.62	0.87
55:B8:1:C:H5'	56:B9:282:LYS:HZ3	1.35	0.86
1:AA:1088:G:H21	1:AA:1167:A:N6	1.74	0.86
1:AA:49:U:C5	1:AA:365:U:O4	2.30	0.85
1:AA:81:A:H2	1:AA:88:U:H3	1.21	0.84
1:AA:208:U:H3	1:AA:211:G:H1	1.24	0.84
1:AA:1026:G:N1	1:AA:1035:A:C5	2.46	0.84
1:AA:49:U:C4	1:AA:365:U:O4	2.31	0.83
1:AA:9:G:OP2	5:AE:126:LYS:NZ	2.13	0.82
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.62	0.82
1:AA:81:A:O2'	1:AA:82:G:N7	2.13	0.82
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.44	0.82
13:AM:7:ILE:HD11	27:BF:112:ARG:HA	1.62	0.81
1:AA:100:G:C5	1:AA:102:G:C5	2.67	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2068:U:H3	22:BA:2430:A:H2	1.25	0.81
22:BA:2103:C:C4	22:BA:2104:C:N4	2.49	0.81
56:B9:117:ARG:HH12	56:B9:362:LYS:HE2	1.46	0.80
6:AF:3:HIS:ND1	6:AF:65:GLU:OE2	2.14	0.80
1:AA:1320:C:OP2	19:AS:3:ARG:NH2	2.15	0.79
1:AA:49:U:O4	1:AA:365:U:O4	2.00	0.79
29:BH:96:THR:HG23	29:BH:115:VAL:HB	1.63	0.79
22:BA:548:G:O2'	22:BA:549:G:O4'	2.01	0.79
22:BA:2611:C:OP2	61:BA:3402:HOH:O	2.00	0.79
1:AA:70:U:O2	1:AA:71:A:N6	2.13	0.79
11:AK:109:ASN:HB3	21:AU:5:LYS:HD3	1.65	0.79
2:AB:122:GLN:NE2	2:AB:123:ASP:OD1	2.17	0.78
22:BA:2840:C:H5"	35:BN:53:THR:HG21	1.64	0.78
55:B8:1:C:H5'	56:B9:282:LYS:HZ1	1.45	0.78
29:BH:97:ARG:HB2	29:BH:112:LYS:HE3	1.66	0.77
47:BZ:6:LYS:NZ	47:BZ:37:GLU:HG3	1.98	0.77
1:AA:1305:G:H21	1:AA:1332:A:H2	1.30	0.77
22:BA:2185:U:O4	22:BA:2186:G:O6	2.02	0.77
22:BA:2639:A:O3'	31:BJ:96:ARG:NH1	2.17	0.77
22:BA:1172:C:N4	22:BA:1178:C:O2	2.17	0.77
30:BI:18:CYS:HB3	30:BI:40:CYS:SG	2.24	0.77
10:AJ:65:TYR:HB3	14:AN:96:LEU:HD11	1.65	0.77
1:AA:81:A:C2	1:AA:88:U:N3	2.51	0.76
22:BA:2185:U:N3	22:BA:2186:G:O6	2.18	0.76
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.49	0.76
23:BB:31:C:O2	23:BB:53:A:N6	2.18	0.76
15:AO:89:ARG:NH2	22:BA:713:G:N7	2.34	0.76
22:BA:285:G:H1	22:BA:355:U:H3	1.32	0.76
22:BA:1250:G:H5"	38:BQ:6:ARG:HD3	1.66	0.76
34:BM:47:GLU:OE1	34:BM:50:ARG:NH1	2.19	0.76
22:BA:2188:U:O2'	22:BA:2189:U:O4'	2.04	0.76
27:BF:80:ARG:HH22	55:B8:56:C:N4	1.84	0.76
1:AA:456:A:H61	1:AA:475:C:H42	1.34	0.75
1:AA:1397:C:OP2	5:AE:29:ARG:NH2	2.19	0.75
1:AA:1350:A:OP2	9:AI:120:LYS:NZ	2.19	0.75
23:BB:1:U:H2'	23:BB:2:G:H8	1.51	0.75
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.19	0.75
7:AG:106:GLU:O	7:AG:110:LYS:NZ	2.20	0.75
22:BA:2141:G:H2'	22:BA:2142:A:H8	1.51	0.75
24:BC:107:PRO:HD2	24:BC:110:LEU:HD22	1.69	0.75
31:BJ:95:ARG:HE	31:BJ:96:ARG:HG3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:358:U:H2'	22:BA:359:G:H8	1.50	0.74
1:AA:85:U:OP2	1:AA:86:G:N2	2.20	0.74
10:AJ:52:LEU:HD11	10:AJ:59:LYS:HA	1.70	0.74
28:BG:164:TYR:HB2	28:BG:167:GLU:HB2	1.66	0.74
8:AH:114:ARG:O	8:AH:118:GLN:NE2	2.21	0.74
5:AE:159:LYS:NZ	8:AH:42:GLU:O	2.20	0.74
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.21	0.74
9:AI:19:VAL:HG22	9:AI:65:ILE:HG12	1.69	0.74
1:AA:100:G:H22	1:AA:152:A:H1'	1.53	0.74
22:BA:280:U:O4	22:BA:360:U:O2	2.05	0.74
13:AM:89:LEU:HD12	13:AM:93:ARG:HH22	1.53	0.73
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.51	0.73
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.70	0.73
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HG12	1.68	0.73
22:BA:2103:C:N4	22:BA:2104:C:N4	2.36	0.73
23:BB:42:C:OP2	30:BI:2:LYS:NZ	2.15	0.73
26:BE:61:ARG:NH2	53:B5:9:THR:OG1	2.22	0.73
1:AA:1130:A:OP1	9:AI:18:ARG:NH2	2.20	0.73
22:BA:2140:G:H1	22:BA:2151:U:H3	1.36	0.73
10:AJ:47:GLU:OE2	14:AN:76:LYS:NZ	2.22	0.73
1:AA:100:G:H2'	1:AA:102:G:H8	1.54	0.72
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.20	0.72
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.22	0.72
4:AD:12:SER:OG	4:AD:17:THR:O	2.07	0.72
1:AA:96:U:H2'	1:AA:97:G:H8	1.55	0.72
22:BA:545:U:O2	22:BA:548:G:N1	2.18	0.72
56:B9:25:LEU:HD21	56:B9:116:ARG:HG3	1.70	0.72
1:AA:635:A:O3'	17:AQ:6:ARG:NH1	2.23	0.72
22:BA:1607:C:N4	22:BA:1622:G:OP2	2.24	0.71
1:AA:68:G:H8	1:AA:69:G:O3'	1.74	0.71
1:AA:746:A:H2'	1:AA:747:A:C8	2.25	0.71
1:AA:97:G:H2'	1:AA:98:A:O4'	1.91	0.71
3:AC:9:GLY:HA2	3:AC:12:LEU:HG	1.72	0.71
27:BF:142:ASP:OD2	27:BF:145:LYS:NZ	2.24	0.71
1:AA:437:U:H5'	4:AD:152:GLN:HE22	1.56	0.71
29:BH:15:LEU:HD21	29:BH:58:LEU:HD11	1.72	0.71
1:AA:840:C:N4	1:AA:842:U:O2'	2.24	0.71
22:BA:1083:U:O2	22:BA:1085:A:N7	2.23	0.71
27:BF:126:GLY:O	27:BF:158:THR:OG1	2.09	0.70
1:AA:68:G:H2'	1:AA:70:U:H5'	1.73	0.70
22:BA:2190:G:H2'	22:BA:2191:A:H8	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1649:G:O2'	35:BN:106:ASP:OD2	2.05	0.70
32:BK:71:ARG:NH2	32:BK:123:LEU:O	2.21	0.70
22:BA:2138:G:O6	22:BA:2154:A:N6	2.25	0.70
22:BA:2831:G:OP2	25:BD:59:ARG:NH2	2.24	0.70
51:B3:32:ILE:H	51:B3:32:ILE:HD12	1.56	0.70
55:B8:18:G:O2'	55:B8:57:G:N2	2.24	0.70
22:BA:884:U:C4	22:BA:892:A:N7	2.60	0.69
22:BA:884:U:O4	22:BA:892:A:N7	2.24	0.69
33:BL:82:LEU:HD22	33:BL:90:VAL:HG21	1.75	0.69
28:BG:2:SER:OG	28:BG:3:ARG:N	2.26	0.69
56:B9:41:LEU:HD21	56:B9:56:LEU:HB3	1.75	0.69
1:AA:202:G:O2'	1:AA:467:U:O4	2.10	0.68
22:BA:2188:U:H2'	22:BA:2189:U:C6	2.28	0.68
56:B9:270:ILE:HD12	56:B9:294:LYS:HG2	1.76	0.68
14:AN:15:LEU:HD23	14:AN:54:ASP:HB2	1.75	0.68
2:AB:82:ASP:OD1	2:AB:83:ALA:N	2.27	0.68
22:BA:1847:A:HO2'	22:BA:1848:A:H8	1.40	0.68
8:AH:96:MET:HG3	8:AH:99:LEU:HB2	1.76	0.68
1:AA:460:A:H2'	1:AA:461:A:C8	2.28	0.68
22:BA:2141:G:H2'	22:BA:2142:A:C8	2.29	0.68
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.27	0.68
1:AA:910:C:OP2	12:AL:18:LYS:NZ	2.26	0.67
14:AN:26:LEU:HD11	14:AN:48:LEU:HD13	1.76	0.67
22:BA:1102:C:H2'	22:BA:1103:A:H8	1.59	0.67
22:BA:2190:G:H2'	22:BA:2191:A:C8	2.29	0.67
22:BA:2261:C:OP1	44:BW:19:LYS:NZ	2.26	0.67
27:BF:140:GLU:OE2	30:BI:26:SER:OG	2.09	0.67
42:BU:89:ASP:OD1	42:BU:90:GLY:N	2.22	0.67
1:AA:96:U:H2'	1:AA:97:G:C8	2.30	0.67
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.28	0.67
56:B9:287:ALA:O	56:B9:291:MET:N	2.28	0.67
22:BA:2102:G:N2	22:BA:2188:U:O2	2.29	0.66
1:AA:100:G:O2'	1:AA:102:G:OP2	2.12	0.66
1:AA:463:U:H2'	1:AA:464:U:C2	2.31	0.66
1:AA:76:G:H1	1:AA:93:U:H3	1.43	0.66
22:BA:1667:G:O2'	22:BA:1991:U:O4	2.12	0.66
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.30	0.66
1:AA:1530:G:O6	21:AU:46:LYS:NZ	2.28	0.66
1:AA:64:G:C2	1:AA:69:G:C4	2.84	0.66
1:AA:102:G:C5	1:AA:103:U:C5	2.83	0.66
9:AI:59:GLU:HG2	9:AI:60:LYS:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:100:G:H2'	1:AA:102:G:C8	2.31	0.66
10:AJ:63:ASP:OD1	14:AN:98:LYS:NZ	2.28	0.66
23:BB:43:C:O2	27:BF:92:ARG:NH2	2.29	0.66
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.28	0.65
2:AB:114:LEU:HD13	2:AB:144:LEU:HD22	1.78	0.65
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.60	0.65
22:BA:1847:A:O2'	22:BA:1848:A:H8	1.79	0.65
22:BA:2611:C:OP2	61:BA:3404:HOH:O	2.14	0.65
22:BA:541:A:N6	22:BA:553:G:O6	2.29	0.65
33:BL:123:ARG:NH1	33:BL:143:GLU:OE1	2.30	0.65
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.31	0.65
9:AI:88:MET:HE1	9:AI:95:ARG:HA	1.78	0.65
19:AS:30:PRO:HA	19:AS:48:THR:HG23	1.79	0.65
22:BA:1729:U:O2'	22:BA:1731:G:N2	2.29	0.65
22:BA:2102:G:H1	22:BA:2188:U:H3	1.44	0.65
22:BA:2377:A:O2'	36:BO:117:PHE:O	2.13	0.65
35:BN:2:ARG:HD2	35:BN:2:ARG:O	1.96	0.65
13:AM:4:ILE:HG22	13:AM:5:ALA:H	1.61	0.64
30:BI:46:GLY:HA2	30:BI:49:ARG:CZ	2.27	0.64
22:BA:2171:A:O2'	22:BA:2173:A:OP1	2.13	0.64
34:BM:62:LYS:HD2	34:BM:64:TRP:CZ2	2.32	0.64
47:BZ:6:LYS:HZ3	47:BZ:37:GLU:HG3	1.62	0.64
56:B9:87:ALA:HA	56:B9:92:ASP:HB3	1.78	0.64
1:AA:100:G:OP1	20:AT:5:LYS:NZ	2.30	0.64
1:AA:102:G:C6	1:AA:103:U:C4	2.86	0.64
8:AH:96:MET:HB3	8:AH:100:GLY:H	1.62	0.64
9:AI:25:ASN:H	9:AI:27:LYS:NZ	1.95	0.64
22:BA:2299:U:OP2	27:BF:71:ARG:NH1	2.30	0.64
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.32	0.64
11:AK:84:VAL:HB	11:AK:110:ILE:HG22	1.80	0.64
22:BA:2113:U:OP2	22:BA:2115:G:N2	2.30	0.64
56:B9:342:THR:HG22	56:B9:344:ASN:H	1.62	0.64
22:BA:2134:A:O2'	22:BA:2135:A:O4'	2.11	0.64
33:BL:62:PRO:HB2	51:B3:30:ARG:HH11	1.63	0.64
2:AB:26:LYS:NZ	2:AB:194:ASP:OD2	2.31	0.64
6:AF:40:GLU:OE1	6:AF:100:SER:OG	2.15	0.64
19:AS:19:VAL:O	19:AS:23:VAL:HG23	1.98	0.64
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.31	0.64
42:BU:4:LYS:O	42:BU:94:ARG:NH2	2.31	0.64
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.61	0.64
34:BM:75:GLU:HG2	34:BM:90:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BU:28:VAL:HG22	42:BU:34:VAL:HG12	1.79	0.64
43:BV:58:SER:O	43:BV:73:LYS:NZ	2.31	0.64
1:AA:100:G:O4'	1:AA:101:A:C8	2.51	0.64
1:AA:100:G:C4	1:AA:102:G:C8	2.86	0.64
2:AB:219:ALA:O	2:AB:222:ARG:N	2.31	0.64
22:BA:534:U:O2'	38:BQ:49:ASP:OD2	2.11	0.64
1:AA:100:G:O2'	1:AA:102:G:O5'	2.16	0.64
41:BT:39:THR:OG1	41:BT:42:GLU:OE1	2.11	0.64
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.31	0.64
22:BA:2305:U:H5"	27:BF:131:GLY:HA3	1.79	0.64
56:B9:358:GLU:N	56:B9:358:GLU:OE1	2.31	0.64
22:BA:1085:A:O2'	22:BA:1086:A:O4'	2.14	0.63
42:BU:34:VAL:HG13	42:BU:67:VAL:HG22	1.79	0.63
1:AA:67:C:C4	1:AA:69:G:C4	2.86	0.63
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.31	0.63
1:AA:28:A:O2'	1:AA:296:U:OP1	2.14	0.63
1:AA:68:G:C8	1:AA:69:G:O3'	2.50	0.63
1:AA:459:A:H2'	1:AA:460:A:C8	2.33	0.63
5:AE:148:ASN:HB2	5:AE:152:MET:SD	2.38	0.63
17:AQ:17:MET:HG3	17:AQ:20:SER:HB2	1.80	0.63
54:B7:1:C:H2'	54:B7:2:G:H8	1.61	0.63
1:AA:67:C:C5	1:AA:69:G:C4	2.87	0.63
22:BA:2161:C:O2'	22:BA:2173:A:O5'	2.16	0.63
56:B9:31:LYS:HA	56:B9:34:LEU:HD12	1.81	0.63
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.34	0.63
56:B9:118:MET:HE1	56:B9:187:TYR:HB3	1.80	0.63
24:BC:133:ARG:CZ	29:BH:123:ARG:HH12	2.12	0.62
56:B9:116:ARG:NH1	56:B9:117:ARG:HG2	2.14	0.62
1:AA:67:C:N4	1:AA:69:G:C2	2.66	0.62
22:BA:946:C:OP2	61:BA:3401:HOH:O	0.62	0.62
48:B0:52:ARG:NH2	48:B0:54:VAL:HG12	2.14	0.62
1:AA:1340:A:HO2'	55:B8:31:G:HO2'	1.47	0.62
22:BA:1101:U:O2'	52:B4:12:ARG:NH2	2.32	0.62
22:BA:2359:C:O2'	51:B3:54:ASP:OD1	2.18	0.62
23:BB:51:G:OP1	36:BO:63:LYS:NZ	2.22	0.62
29:BH:5:LEU:HD13	29:BH:17:ASP:HB2	1.82	0.62
22:BA:884:U:O4	22:BA:892:A:C6	2.52	0.62
1:AA:1350:A:O2'	7:AG:33:ASP:OD1	2.17	0.62
22:BA:1065:U:H3	22:BA:1073:A:H61	1.47	0.62
22:BA:2116:G:N7	22:BA:2165:C:N4	2.47	0.62
2:AB:114:LEU:HB2	2:AB:144:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2799:A:O2'	22:BA:2800:A:H5"	2.00	0.62
16:AP:48:GLU:HG3	16:AP:49:GLY:H	1.63	0.62
22:BA:2109:U:O2	22:BA:2180:U:O4	2.17	0.62
56:B9:22:ARG:HE	56:B9:70:LEU:HD13	1.65	0.62
7:AG:138:ARG:NH2	7:AG:139:GLU:OE2	2.31	0.61
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.31	0.61
1:AA:1180:A:OP2	9:AI:99:ARG:NH2	2.32	0.61
22:BA:1753:G:OP1	37:BP:93:ARG:NH1	2.34	0.61
1:AA:492:C:H2'	1:AA:493:A:C8	2.34	0.61
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.26	0.61
6:AF:44:ARG:HD2	6:AF:56:LYS:HG3	1.81	0.61
1:AA:68:G:C6	1:AA:100:G:O6	2.54	0.61
46:BY:10:SER:OG	46:BY:13:GLU:OE1	2.16	0.61
9:AI:12:ARG:HG3	9:AI:13:LYS:H	1.65	0.61
22:BA:2134:A:H1'	22:BA:2159:G:H1'	1.83	0.61
1:AA:64:G:C4	1:AA:69:G:C6	2.89	0.61
22:BA:1914:C:N4	56:B9:315:SER:O	2.24	0.61
56:B9:170:GLU:HA	56:B9:176:ILE:HA	1.81	0.61
3:AC:49:LYS:O	3:AC:72:ARG:NH1	2.34	0.61
7:AG:118:LEU:O	7:AG:122:ASN:ND2	2.33	0.61
22:BA:358:U:H2'	22:BA:359:G:C8	2.33	0.61
29:BH:82:SER:HB2	29:BH:90:LEU:HD11	1.82	0.61
56:B9:333:ILE:HG13	56:B9:345:THR:HG22	1.82	0.61
1:AA:382:A:H2'	1:AA:383:A:C8	2.36	0.61
5:AE:163:GLU:HB3	8:AH:114:ARG:HH22	1.65	0.61
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.81	0.61
41:BT:56:GLU:N	41:BT:56:GLU:OE1	2.33	0.61
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.32	0.61
9:AI:46:MET:O	9:AI:50:GLN:HG3	2.01	0.61
11:AK:108:THR:O	21:AU:6:VAL:HG12	2.01	0.61
22:BA:2316:G:H2'	22:BA:2317:A:H8	1.66	0.61
29:BH:84:ALA:HB2	29:BH:90:LEU:HD12	1.83	0.61
1:AA:673:A:H2'	1:AA:674:G:C8	2.36	0.60
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.35	0.60
22:BA:2118:U:O2	22:BA:2145:C:N4	2.34	0.60
41:BT:1:MET:HG2	41:BT:2:ILE:N	2.16	0.60
1:AA:462:G:C5	1:AA:463:U:C4	2.89	0.60
1:AA:481:G:O2'	1:AA:483:C:N4	2.34	0.60
9:AI:129:LYS:NZ	55:B8:34:C:OP2	2.27	0.60
22:BA:883:G:H1	22:BA:894:U:HO2'	1.47	0.60
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BI:11:GLU:OE2	30:BI:23:LYS:HD2	2.01	0.60
22:BA:2180:U:H2'	22:BA:2181:U:H6	1.66	0.60
56:B9:69:THR:HG23	56:B9:109:LYS:HE3	1.83	0.60
1:AA:100:G:C6	1:AA:102:G:C4	2.89	0.60
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.66	0.60
4:AD:58:LYS:NZ	4:AD:69:GLU:OE1	2.34	0.60
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.17	0.60
26:BE:168:ASP:OD2	26:BE:170:ARG:NH1	2.31	0.60
1:AA:458:U:H2'	1:AA:459:A:C8	2.36	0.60
2:AB:114:LEU:HB2	2:AB:144:LEU:HD22	1.84	0.60
22:BA:2365:G:N7	51:B3:39:LYS:NZ	2.47	0.60
34:BM:20:LEU:HD13	43:BV:81:PRO:HG2	1.84	0.60
51:B3:31:HIS:C	51:B3:33:LEU:H	2.05	0.60
56:B9:74:LYS:O	56:B9:78:GLU:HG3	2.02	0.60
22:BA:636:G:OP1	33:BL:129:LYS:NZ	2.32	0.60
1:AA:337:G:H2'	1:AA:338:A:C8	2.36	0.60
5:AE:153:VAL:HG23	5:AE:156:LYS:HE3	1.84	0.60
22:BA:881:G:N2	22:BA:895:U:O2	2.34	0.60
56:B9:15:THR:HA	56:B9:77:LEU:HD13	1.83	0.60
1:AA:171:A:H2'	1:AA:172:A:C8	2.37	0.59
10:AJ:36:VAL:HG22	10:AJ:76:ILE:HD12	1.82	0.59
22:BA:1022:G:O6	31:BJ:68:LYS:NZ	2.30	0.59
3:AC:110:GLU:HB2	3:AC:144:LEU:HD12	1.83	0.59
1:AA:147:G:H2'	1:AA:148:G:C8	2.37	0.59
22:BA:1064:C:H2'	22:BA:1065:U:C6	2.38	0.59
22:BA:2103:C:N4	22:BA:2104:C:H41	1.95	0.59
29:BH:135:HIS:HB3	29:BH:138:VAL:HG22	1.84	0.59
36:BO:50:ALA:O	36:BO:81:ARG:NH2	2.35	0.59
5:AE:161:VAL:HG22	5:AE:162:GLU:H	1.67	0.59
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.17	0.59
4:AD:174:ASP:OD2	4:AD:177:LYS:NZ	2.35	0.59
11:AK:111:THR:HG23	21:AU:3:VAL:HB	1.83	0.59
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	1.84	0.59
41:BT:11:LEU:O	46:BY:29:ARG:NH1	2.34	0.59
1:AA:72:A:H2'	1:AA:73:C:O4'	2.03	0.59
1:AA:235:C:H2'	1:AA:236:A:C8	2.38	0.59
1:AA:1316:G:N2	1:AA:1318:A:H3'	2.17	0.59
22:BA:585:G:N7	38:BQ:6:ARG:NH1	2.51	0.59
34:BM:78:LEU:HD12	56:B9:281:HIS:CD2	2.38	0.59
1:AA:1250:A:H2'	1:AA:1251:A:C8	2.38	0.59
22:BA:884:U:N3	22:BA:892:A:C8	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
2:AB:32:PHE:HB2	2:AB:42:ASN:HB2	1.85	0.59
55:B8:2:G:O2'	55:B8:3:G:H2'	2.02	0.59
14:AN:32:ASP:OD1	14:AN:33:VAL:N	2.36	0.58
1:AA:126:G:OP1	1:AA:605:U:O2'	2.19	0.58
14:AN:29:ILE:HG13	14:AN:30:ILE:HD12	1.85	0.58
1:AA:79:G:H2'	1:AA:80:A:C8	2.38	0.58
1:AA:79:G:H2'	1:AA:80:A:H8	1.69	0.58
1:AA:100:G:O2'	1:AA:102:G:P	2.61	0.58
1:AA:713:G:H2'	1:AA:714:G:C8	2.38	0.58
1:AA:457:G:N2	1:AA:475:C:C2	2.72	0.58
1:AA:1026:G:O6	1:AA:1035:A:N6	2.37	0.58
22:BA:1156:A:C8	38:BQ:51:ARG:HG2	2.39	0.58
22:BA:1798:U:OP2	24:BC:271:ARG:NH2	2.36	0.58
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.52	0.58
2:AB:54:LEU:HG	2:AB:220:THR:HG21	1.85	0.58
14:AN:46:LEU:HD11	19:AS:13:LEU:HD13	1.85	0.58
22:BA:2798:U:H4'	22:BA:2799:A:H5'	1.86	0.58
51:B3:31:HIS:ND1	51:B3:32:ILE:HD12	2.19	0.58
1:AA:64:G:C2	1:AA:70:U:C4	2.91	0.58
22:BA:2100:G:H3'	22:BA:2101:A:H8	1.69	0.58
22:BA:2250:G:O2'	22:BA:2496:C:OP1	2.22	0.58
26:BE:6:LYS:HB3	26:BE:121:VAL:HG12	1.85	0.58
50:B2:24:THR:HG23	50:B2:27:GLY:H	1.68	0.58
1:AA:1038:C:H2'	1:AA:1039:G:H8	1.68	0.58
22:BA:2327:A:H2'	22:BA:2328:A:C8	2.38	0.58
56:B9:80:VAL:HG11	56:B9:103:LEU:HD13	1.84	0.58
1:AA:76:G:C4	1:AA:77:A:C8	2.92	0.58
31:BJ:95:ARG:HH21	31:BJ:96:ARG:HD2	1.68	0.58
1:AA:632:U:H5"	1:AA:633:G:C8	2.39	0.57
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.39	0.57
49:B1:29:THR:HG23	49:B1:30:LYS:HG2	1.84	0.57
1:AA:465:A:O2'	1:AA:466:A:O4'	2.19	0.57
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.13	0.57
22:BA:597:G:O2'	33:BL:11:GLY:O	2.21	0.57
1:AA:469:C:H2'	1:AA:470:C:C6	2.39	0.57
1:AA:1491:G:H5'	1:AA:1492:A:OP2	2.04	0.57
25:BD:46:ARG:NH1	25:BD:85:ALA:O	2.37	0.57
56:B9:7:VAL:HG23	56:B9:8:ASN:H	1.68	0.57
56:B9:15:THR:O	56:B9:18:SER:OG	2.19	0.57
22:BA:1086:A:O2'	22:BA:1087:G:N7	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BZ:40:ASP:OD1	47:BZ:45:ARG:HD3	2.03	0.57
1:AA:68:G:H5'	1:AA:171:A:H1'	1.87	0.57
1:AA:524:G:H2'	1:AA:525:C:C6	2.39	0.57
22:BA:2139:U:H2'	22:BA:2140:G:C8	2.40	0.57
40:BS:66:ILE:H	40:BS:66:ILE:HD12	1.69	0.57
56:B9:22:ARG:NE	56:B9:70:LEU:HD13	2.19	0.57
22:BA:278:A:H2	22:BA:361:G:N3	2.03	0.57
27:BF:56:ASP:OD1	27:BF:57:LEU:N	2.38	0.57
1:AA:68:G:OP2	1:AA:69:G:H4'	2.05	0.57
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.69	0.57
2:AB:210:VAL:HA	2:AB:213:TYR:HD2	1.70	0.57
22:BA:871:U:H2'	22:BA:872:U:C6	2.40	0.57
26:BE:2:GLU:OE2	26:BE:12:LEU:N	2.38	0.57
27:BF:98:GLU:OE2	30:BI:25:ARG:HD3	2.04	0.57
56:B9:28:ASP:O	56:B9:32:GLU:N	2.32	0.57
56:B9:265:HIS:CD2	56:B9:267:PRO:HD2	2.40	0.57
34:BM:42:THR:HG22	34:BM:44:ARG:H	1.70	0.57
56:B9:243:VAL:HG12	56:B9:261:VAL:HG12	1.87	0.57
22:BA:857:G:H2'	22:BA:858:G:O4'	2.05	0.57
22:BA:2104:C:H2'	22:BA:2105:U:C6	2.39	0.57
24:BC:142:HIS:ND1	24:BC:193:GLY:O	2.35	0.57
1:AA:728:A:H2'	1:AA:729:A:C8	2.40	0.56
22:BA:1082:U:H2'	22:BA:1083:U:C6	2.39	0.56
1:AA:49:U:O4	1:AA:365:U:C4	2.59	0.56
1:AA:67:C:C6	1:AA:69:G:H1'	2.41	0.56
9:AI:91:ASP:OD1	9:AI:92:GLU:N	2.37	0.56
22:BA:1292:G:H2'	22:BA:1293:C:C6	2.40	0.56
24:BC:16:VAL:HG22	24:BC:206:GLY:HA3	1.86	0.56
1:AA:49:U:H5	1:AA:365:U:O4	1.86	0.56
1:AA:78:A:H2'	1:AA:79:G:C8	2.41	0.56
1:AA:100:G:C5	1:AA:101:A:C6	2.93	0.56
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.40	0.56
22:BA:2170:A:H1'	22:BA:2171:A:C8	2.40	0.56
56:B9:94:GLU:O	56:B9:98:GLU:N	2.32	0.56
1:AA:70:U:H1'	1:AA:71:A:N7	2.20	0.56
2:AB:23:TRP:HZ3	2:AB:25:PRO:HA	1.70	0.56
56:B9:83:LEU:HB3	56:B9:95:THR:HG21	1.87	0.56
8:AH:38:ASN:O	8:AH:41:LYS:N	2.36	0.56
20:AT:36:TYR:O	20:AT:39:ILE:N	2.39	0.56
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.40	0.56
22:BA:2107:G:H2'	22:BA:2108:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:100:G:C6	1:AA:102:G:C5	2.93	0.56
1:AA:208:U:O2	1:AA:211:G:O6	2.23	0.56
1:AA:64:G:N3	1:AA:69:G:C5	2.74	0.56
1:AA:87:C:H2'	1:AA:88:U:H4'	1.87	0.56
1:AA:1124:G:H4'	10:AJ:40:ILE:HD11	1.88	0.56
3:AC:114:LYS:HB2	3:AC:185:ASN:HD22	1.71	0.56
22:BA:2661:G:H2'	22:BA:2662:A:C8	2.41	0.56
26:BE:10:SER:OG	26:BE:11:ALA:N	2.39	0.56
39:BR:37:GLU:O	39:BR:37:GLU:HG2	2.06	0.56
56:B9:230:ILE:HG23	56:B9:299:GLU:HG2	1.86	0.56
22:BA:1729:U:O2	22:BA:1731:G:N2	2.36	0.56
41:BT:2:ILE:HD13	41:BT:42:GLU:HG3	1.87	0.56
8:AH:39:VAL:HG21	8:AH:110:VAL:HG12	1.88	0.55
14:AN:26:LEU:HA	14:AN:30:ILE:HD13	1.86	0.55
22:BA:2331:G:OP1	44:BW:44:LYS:NZ	2.39	0.55
22:BA:1278:C:H2'	22:BA:1279:G:H8	1.71	0.55
22:BA:1738:G:O2'	22:BA:1739:A:H8	1.89	0.55
22:BA:1870:C:H2'	22:BA:1871:A:C8	2.41	0.55
22:BA:703:U:H2'	22:BA:704:G:O4'	2.05	0.55
1:AA:64:G:N2	1:AA:69:G:H2'	2.21	0.55
1:AA:469:C:H2'	1:AA:470:C:H6	1.71	0.55
22:BA:1178:C:H2'	22:BA:1179:G:H8	1.72	0.55
31:BJ:21:THR:HG22	31:BJ:61:LYS:HD2	1.88	0.55
32:BK:40:LYS:HD3	32:BK:58:LEU:O	2.06	0.55
37:BP:34:GLU:OE2	37:BP:39:ARG:NE	2.39	0.55
40:BS:12:SER:O	40:BS:101:SER:OG	2.22	0.55
56:B9:33:ARG:HD2	56:B9:63:LEU:HD21	1.87	0.55
1:AA:71:A:C2	1:AA:101:A:C5	2.94	0.55
1:AA:933:G:OP1	7:AG:4:ARG:NH1	2.38	0.55
1:AA:279:A:C8	1:AA:279:A:H5'	2.41	0.55
1:AA:279:A:H5'	1:AA:279:A:H8	1.71	0.55
1:AA:662:U:H2'	1:AA:663:A:C8	2.41	0.55
1:AA:714:G:H2'	1:AA:715:A:C8	2.41	0.55
22:BA:1980:G:O2'	22:BA:1982:U:OP2	2.24	0.55
24:BC:181:MET:HB2	24:BC:268:VAL:HB	1.89	0.55
22:BA:552:U:H2'	22:BA:553:G:H8	1.71	0.55
22:BA:2140:G:H2'	22:BA:2141:G:O4'	2.07	0.55
56:B9:330:ASP:OD2	56:B9:332:ARG:NH1	2.39	0.55
1:AA:100:G:C6	1:AA:102:G:C2	2.95	0.55
1:AA:718:A:C2	18:AR:38:LYS:HE2	2.41	0.55
11:AK:31:ILE:HG23	11:AK:46:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BD:133:THR:HG22	25:BD:134:HIS:H	1.72	0.55
51:B3:32:ILE:HG22	51:B3:32:ILE:O	2.05	0.55
2:AB:43:LEU:HA	2:AB:46:THR:HG22	1.88	0.55
22:BA:545:U:O2'	22:BA:546:U:O4'	2.24	0.55
37:BP:2:SER:O	37:BP:2:SER:OG	2.24	0.55
22:BA:1614:A:C2	40:BS:93:ALA:HB2	2.42	0.55
1:AA:100:G:C5	1:AA:102:G:C4	2.95	0.54
3:AC:186:THR:HG23	3:AC:199:LYS:HG2	1.89	0.54
5:AE:116:GLU:OE2	5:AE:117:VAL:HG23	2.06	0.54
41:BT:33:LYS:HG3	41:BT:80:TRP:CE3	2.42	0.54
55:B8:46:G:H2'	55:B8:47:U:H5'	1.89	0.54
56:B9:8:ASN:HA	56:B9:11:ILE:HD12	1.89	0.54
1:AA:1179:A:OP2	9:AI:99:ARG:NH1	2.40	0.54
22:BA:848:C:H2'	22:BA:849:A:C8	2.42	0.54
22:BA:2068:U:N3	22:BA:2430:A:H2	2.01	0.54
27:BF:140:GLU:HA	30:BI:28:VAL:HG22	1.89	0.54
32:BK:12:ASP:OD2	32:BK:14:SER:OG	2.25	0.54
1:AA:73:C:C2	1:AA:74:A:C8	2.95	0.54
27:BF:110:ARG:HH22	27:BF:139:PRO:HB3	1.73	0.54
51:B3:31:HIS:O	51:B3:33:LEU:N	2.39	0.54
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.42	0.54
6:AF:3:HIS:HB2	6:AF:92:THR:O	2.08	0.54
22:BA:996:A:O3'	38:BQ:91:ASP:OD1	2.26	0.54
1:AA:81:A:H2	1:AA:88:U:N3	1.97	0.54
1:AA:91:U:H2'	1:AA:92:U:C6	2.43	0.54
3:AC:135:LYS:HD3	3:AC:168:TYR:CD2	2.42	0.54
22:BA:2100:G:C5	22:BA:2101:A:C5	2.95	0.54
22:BA:2152:G:H2'	22:BA:2153:C:C6	2.42	0.54
31:BJ:140:LEU:HG	31:BJ:142:ILE:HB	1.88	0.54
1:AA:1492:A:H5'	12:AL:44:LYS:HD2	1.88	0.54
22:BA:2130:U:O2'	22:BA:2133:G:O2'	2.24	0.54
22:BA:2191:A:H2'	22:BA:2192:U:C6	2.42	0.54
29:BH:7:ASP:OD1	29:BH:8:LYS:N	2.40	0.54
22:BA:1177:G:H2'	22:BA:1178:C:C6	2.42	0.54
30:BI:30:HIS:CG	30:BI:31:ASP:H	2.26	0.54
3:AC:79:LYS:HD2	3:AC:80:LYS:HG3	1.89	0.54
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.72	0.54
22:BA:634:C:H2'	22:BA:635:C:C6	2.43	0.54
56:B9:288:MET:HG3	56:B9:289:LYS:HD2	1.90	0.54
1:AA:66:A:C6	1:AA:67:C:C5	2.96	0.54
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AQ:12:VAL:HG23	17:AQ:59:VAL:HG21	1.90	0.54
29:BH:9:VAL:HG11	29:BH:12:LEU:HD12	1.90	0.54
53:B5:11:LYS:HD2	53:B5:13:PHE:CZ	2.43	0.54
28:BG:25:THR:OG1	28:BG:32:GLU:OE2	2.26	0.54
3:AC:16:LYS:NZ	3:AC:181:ASP:OD1	2.41	0.53
12:AL:45:PRO:HB2	54:B7:10:U:N3	2.22	0.53
22:BA:2102:G:H2'	22:BA:2103:C:O4'	2.08	0.53
28:BG:86:LYS:HG2	28:BG:132:VAL:HG12	1.90	0.53
19:AS:4:SER:OG	19:AS:5:LEU:N	2.41	0.53
19:AS:42:PRO:HD3	30:BI:60:PHE:CE2	2.43	0.53
22:BA:1292:G:H2'	22:BA:1293:C:H6	1.72	0.53
22:BA:2876:G:OP1	37:BP:2:SER:N	2.41	0.53
33:BL:73:ILE:HB	33:BL:106:GLU:OE1	2.08	0.53
37:BP:88:ARG:NH2	37:BP:110:ILE:O	2.37	0.53
1:AA:1035:A:H2'	1:AA:1035:A:N3	2.22	0.53
34:BM:50:ARG:HG3	34:BM:65:ILE:HD11	1.89	0.53
1:AA:215:C:H2'	1:AA:216:U:C6	2.44	0.53
6:AF:44:ARG:HB3	6:AF:56:LYS:HE3	1.89	0.53
22:BA:2204:G:OP2	24:BC:147:LYS:NZ	2.34	0.53
54:B7:2:G:N2	54:B7:3:C:O4'	2.40	0.53
1:AA:98:A:H2'	1:AA:99:C:O4'	2.09	0.53
1:AA:389:A:H3'	1:AA:390:U:H6	1.74	0.53
6:AF:42:TRP:CH2	6:AF:102:MET:HG3	2.44	0.53
7:AG:65:ALA:HB2	7:AG:128:ALA:HB2	1.91	0.53
22:BA:2267:A:H5"	22:BA:2268:A:H5'	1.89	0.53
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.91	0.53
16:AP:55:ASP:OD1	16:AP:56:ARG:N	2.42	0.53
1:AA:1229:A:O2'	55:B8:30:C:OP1	2.27	0.53
19:AS:18:LYS:HD3	19:AS:31:LEU:HD11	1.91	0.53
22:BA:364:C:H2'	22:BA:365:U:C6	2.43	0.53
55:B8:71:C:H2'	55:B8:72:G:C8	2.44	0.53
1:AA:539:A:H2'	1:AA:540:G:C8	2.44	0.53
22:BA:404:A:N6	22:BA:421:C:O2'	2.41	0.53
27:BF:115:ARG:O	30:BI:47:LYS:NZ	2.42	0.53
46:BY:10:SER:H	46:BY:13:GLU:CD	2.12	0.53
56:B9:353:LEU:O	56:B9:357:ILE:HG12	2.08	0.53
1:AA:100:G:N2	1:AA:152:A:H1'	2.22	0.53
1:AA:1317:C:O2	19:AS:37:ARG:NH2	2.37	0.53
3:AC:72:ARG:O	3:AC:75:ILE:HG22	2.09	0.53
1:AA:70:U:H6	1:AA:70:U:O5'	1.93	0.52
1:AA:71:A:N1	1:AA:72:A:C5	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.44	0.52
41:BT:28:ASN:ND2	41:BT:88:LYS:O	2.42	0.52
11:AK:59:THR:HG22	11:AK:61:PHE:H	1.75	0.52
13:AM:66:GLU:O	13:AM:69:LEU:N	2.43	0.52
22:BA:1202:G:O6	22:BA:1244:A:N6	2.42	0.52
39:BR:5:PHE:HB3	39:BR:59:ILE:HD12	1.91	0.52
1:AA:738:C:OP1	6:AF:2:ARG:NH2	2.43	0.52
3:AC:56:VAL:HG22	3:AC:67:THR:HB	1.92	0.52
5:AE:115:LEU:HD13	5:AE:123:VAL:HG11	1.92	0.52
7:AG:143:ARG:O	7:AG:146:GLU:HG3	2.09	0.52
19:AS:6:LYS:NZ	30:BI:63:ARG:HD3	2.24	0.52
22:BA:1072:C:N4	22:BA:1093:G:O6	2.43	0.52
22:BA:1149:G:H2'	22:BA:1150:C:C6	2.45	0.52
23:BB:43:C:H5"	30:BI:1:MET:SD	2.50	0.52
56:B9:195:GLU:OE1	56:B9:324:ARG:NH1	2.42	0.52
1:AA:70:U:C5	1:AA:94:G:C8	2.97	0.52
7:AG:111:ARG:HB2	7:AG:119:ARG:HG3	1.91	0.52
10:AJ:7:ARG:NH2	10:AJ:75:ASP:OD2	2.43	0.52
22:BA:181:A:H2'	22:BA:182:A:C8	2.45	0.52
22:BA:2185:U:N3	22:BA:2186:G:C6	2.78	0.52
22:BA:2284:A:OP1	49:B1:5:ILE:HB	2.10	0.52
22:BA:500:G:N1	22:BA:503:A:OP2	2.40	0.52
22:BA:639:U:H2'	22:BA:640:C:C6	2.44	0.52
22:BA:2110:G:H8	22:BA:2110:G:OP2	1.92	0.52
24:BC:29:PRO:HG2	24:BC:34:LEU:HD11	1.91	0.52
31:BJ:19:ASP:OD2	31:BJ:58:ASN:ND2	2.42	0.52
1:AA:972:C:OP2	10:AJ:59:LYS:NZ	2.39	0.52
11:AK:35:THR:HG22	11:AK:41:ALA:HA	1.91	0.52
22:BA:2101:A:H2'	22:BA:2102:G:C8	2.45	0.52
22:BA:2191:A:H2'	22:BA:2192:U:H6	1.75	0.52
22:BA:2316:G:H2'	22:BA:2317:A:C8	2.44	0.52
41:BT:55:VAL:HG12	41:BT:87:LEU:HD23	1.91	0.52
1:AA:68:G:C8	1:AA:69:G:O2'	2.60	0.52
4:AD:44:ARG:HG3	4:AD:46:PRO:HD3	1.92	0.52
22:BA:483:A:OP1	42:BU:47:LYS:NZ	2.39	0.52
22:BA:1073:A:H4'	22:BA:2474:U:H4'	1.91	0.52
48:B0:53:LYS:HE3	48:B0:56:ALA:HA	1.92	0.52
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.45	0.52
22:BA:1746:A:H2'	22:BA:1747:U:C6	2.45	0.52
23:BB:106:G:H2'	23:BB:107:G:O4'	2.10	0.52
56:B9:65:ALA:O	56:B9:69:THR:OG1	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:87:ALA:HB1	56:B9:96:PHE:HB2	1.92	0.52
1:AA:457:G:N2	1:AA:474:G:H22	2.08	0.52
1:AA:461:A:H2'	1:AA:462:G:C8	2.45	0.52
1:AA:1147:C:O2	9:AI:18:ARG:NH1	2.43	0.52
22:BA:1172:C:H5"	22:BA:1173:U:C2	2.45	0.52
22:BA:1494:A:H2'	22:BA:1495:A:C8	2.45	0.52
22:BA:2163:A:H3'	22:BA:2164:C:H4'	1.91	0.52
22:BA:2728:U:HO2'	22:BA:2729:G:H8	1.58	0.52
47:BZ:6:LYS:HZ1	47:BZ:37:GLU:HG3	1.73	0.52
1:AA:191:G:H2'	1:AA:192:A:C8	2.45	0.52
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.45	0.52
1:AA:1507:A:H2'	1:AA:1508:A:C8	2.44	0.52
5:AE:11:LEU:HD23	5:AE:39:VAL:HG22	1.92	0.52
27:BF:147:ASP:N	27:BF:147:ASP:OD1	2.40	0.52
47:BZ:37:GLU:O	47:BZ:38:ARG:NH1	2.42	0.52
22:BA:1102:C:C2	22:BA:1103:A:C8	2.98	0.51
1:AA:208:U:O4	1:AA:211:G:N2	2.36	0.51
1:AA:908:A:H2'	1:AA:909:A:C8	2.45	0.51
17:AQ:79:VAL:HG23	17:AQ:80:GLU:OE1	2.10	0.51
22:BA:172:A:H2'	22:BA:173:A:H8	1.75	0.51
22:BA:882:G:N2	22:BA:883:G:O6	2.43	0.51
29:BH:61:VAL:O	29:BH:65:ALA:N	2.39	0.51
51:B3:31:HIS:O	51:B3:33:LEU:HG	2.10	0.51
1:AA:100:G:N9	1:AA:102:G:C8	2.79	0.51
1:AA:166:U:H2'	1:AA:167:A:H8	1.75	0.51
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.10	0.51
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.43	0.51
2:AB:57:LEU:HD21	2:AB:217:VAL:HG13	1.91	0.51
6:AF:73:GLU:HA	6:AF:76:THR:HB	1.93	0.51
12:AL:79:VAL:N	12:AL:103:ASP:OD2	2.41	0.51
22:BA:849:A:H2'	22:BA:850:U:C6	2.45	0.51
44:BW:26:PHE:H	44:BW:29:GLU:HG3	1.74	0.51
1:AA:384:G:H2'	1:AA:385:C:C6	2.45	0.51
1:AA:1007:U:O2'	1:AA:1008:U:H5'	2.11	0.51
4:AD:58:LYS:HD2	4:AD:204:TYR:OH	2.11	0.51
22:BA:281:C:H2'	22:BA:282:A:C8	2.46	0.51
22:BA:881:G:H21	22:BA:896:A:N6	2.08	0.51
22:BA:2020:A:H5'	48:B0:9:THR:CG2	2.40	0.51
29:BH:99:ILE:HD11	29:BH:122:LEU:HD11	1.91	0.51
13:AM:68:ASP:OD1	13:AM:69:LEU:N	2.43	0.51
22:BA:414:C:H2'	22:BA:415:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BD:12:THR:OG1	37:BP:9:GLU:OE2	2.17	0.51
55:B8:66:A:H2'	55:B8:67:U:C6	2.46	0.51
1:AA:100:G:N1	1:AA:102:G:N3	2.58	0.51
1:AA:142:G:H3'	1:AA:143:A:H8	1.76	0.51
1:AA:555:U:H2'	1:AA:556:C:C6	2.46	0.51
22:BA:587:C:C2	33:BL:19:LEU:HD12	2.46	0.51
55:B8:62:C:H2'	55:B8:63:U:C6	2.45	0.51
1:AA:92:U:H2'	1:AA:93:U:C6	2.44	0.51
22:BA:2101:A:H2'	22:BA:2102:G:O4'	2.11	0.51
22:BA:2102:G:C2	22:BA:2103:C:H1'	2.46	0.51
22:BA:2125:G:N1	22:BA:2171:A:OP1	2.36	0.51
1:AA:486:U:H2'	1:AA:487:A:H8	1.75	0.51
13:AM:3:ARG:NH2	13:AM:7:ILE:HB	2.26	0.51
22:BA:2305:U:H2'	22:BA:2306:C:C6	2.46	0.51
38:BQ:58:ARG:O	38:BQ:62:ILE:HG12	2.11	0.51
1:AA:1207:2MG:HM23	1:AA:1208:C:H1'	1.93	0.51
5:AE:161:VAL:HG13	5:AE:163:GLU:OE1	2.11	0.51
22:BA:1085:A:H2'	22:BA:1086:A:C4	2.46	0.51
22:BA:2151:U:H2'	22:BA:2152:G:C8	2.46	0.51
23:BB:1:U:H2'	23:BB:2:G:C8	2.39	0.51
29:BH:97:ARG:HE	29:BH:112:LYS:HZ1	1.57	0.51
51:B3:62:LEU:HB3	51:B3:65:ALA:HB2	1.93	0.51
53:B5:8:VAL:HG22	53:B5:9:THR:H	1.76	0.51
56:B9:99:ALA:O	56:B9:103:LEU:N	2.34	0.51
1:AA:66:A:C6	1:AA:67:C:C4	2.99	0.51
1:AA:78:A:H2'	1:AA:79:G:H8	1.76	0.51
1:AA:166:U:H2'	1:AA:167:A:C8	2.46	0.51
1:AA:1151:A:H5"	10:AJ:44:THR:HG23	1.93	0.51
2:AB:8:ASP:OD1	2:AB:8:ASP:N	2.40	0.51
12:AL:55:VAL:HG11	12:AL:80:ILE:HD11	1.93	0.51
14:AN:92:GLU:N	14:AN:92:GLU:OE1	2.44	0.51
22:BA:2180:U:H2'	22:BA:2181:U:C6	2.45	0.51
22:BA:2343:U:HO2'	22:BA:2373:G:HO2'	1.55	0.51
34:BM:136:MET:SD	43:BV:76:ASP:HA	2.51	0.51
37:BP:27:GLU:HG3	37:BP:87:LYS:HE2	1.93	0.51
1:AA:632:U:H5"	1:AA:633:G:H8	1.76	0.50
1:AA:1297:G:N2	7:AG:114:LYS:HB3	2.26	0.50
22:BA:1092:C:H2'	22:BA:1093:G:C8	2.46	0.50
40:BS:1:MET:SD	40:BS:3:THR:OG1	2.69	0.50
7:AG:18:PHE:CZ	7:AG:58:GLU:HG2	2.46	0.50
7:AG:135:VAL:O	7:AG:139:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:248:G:H5'	22:BA:250:G:N7	2.26	0.50
22:BA:748:G:C8	40:BS:89:ALA:HB1	2.46	0.50
22:BA:2143:C:H2'	22:BA:2144:G:O4'	2.11	0.50
24:BC:35:GLU:HG2	24:BC:36:LYS:H	1.75	0.50
37:BP:5:ILE:O	37:BP:9:GLU:HG2	2.10	0.50
1:AA:83:C:O2'	1:AA:85:U:N3	2.41	0.50
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.46	0.50
5:AE:105:ILE:HD13	5:AE:116:GLU:HB3	1.93	0.50
6:AF:37:HIS:CD2	6:AF:65:GLU:HG2	2.46	0.50
22:BA:1485:U:H2'	22:BA:1486:U:H6	1.77	0.50
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.46	0.50
43:BV:51:GLN:OE1	43:BV:57:TYR:OH	2.29	0.50
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.76	0.50
16:AP:47:GLU:HG2	16:AP:48:GLU:O	2.11	0.50
56:B9:200:ARG:NE	56:B9:322:GLN:OE1	2.44	0.50
1:AA:1118:U:OP1	9:AI:11:ARG:HD2	2.11	0.50
22:BA:1073:A:O5'	22:BA:1073:A:H8	1.95	0.50
22:BA:2101:A:N1	22:BA:2102:G:C6	2.80	0.50
22:BA:2683:C:O2	32:BK:70:ARG:NH2	2.44	0.50
25:BD:90:PHE:HD2	25:BD:94:GLN:NE2	2.09	0.50
27:BF:80:ARG:HH22	55:B8:56:C:H42	1.56	0.50
28:BG:175:LYS:HE2	28:BG:177:LYS:HB3	1.94	0.50
30:BI:36:VAL:HG11	30:BI:41:HIS:HD2	1.76	0.50
1:AA:100:G:C6	1:AA:102:G:C6	2.99	0.50
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.47	0.50
7:AG:42:ILE:HD12	7:AG:116:MET:HB3	1.94	0.50
22:BA:1847:A:O2'	22:BA:1848:A:C8	2.55	0.50
4:AD:101:VAL:HG11	4:AD:137:VAL:HG21	1.94	0.50
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.44	0.50
22:BA:728:G:H4'	24:BC:13:ARG:HD3	1.94	0.50
27:BF:102:ARG:HG3	30:BI:24:ILE:HD11	1.94	0.50
30:BI:30:HIS:CG	30:BI:31:ASP:N	2.80	0.50
1:AA:1130:A:O2'	9:AI:5:GLN:NE2	2.40	0.50
5:AE:153:VAL:HG11	8:AH:99:LEU:HD22	1.94	0.50
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.47	0.50
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.46	0.50
46:BY:3:ALA:HB2	46:BY:52:ARG:HD3	1.93	0.50
1:AA:68:G:OP2	1:AA:69:G:O5'	2.30	0.50
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.29	0.50
1:AA:1029:U:H3'	1:AA:1031:C:C6	2.46	0.50
19:AS:64:ASP:OD2	19:AS:65:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.47	0.50
22:BA:2014:A:H2'	22:BA:2015:A:C8	2.47	0.50
24:BC:35:GLU:HG2	24:BC:36:LYS:N	2.27	0.50
56:B9:129:TYR:HE1	56:B9:225:GLU:HG3	1.76	0.50
1:AA:633:G:H2'	1:AA:634:C:H6	1.76	0.49
13:AM:12:HIS:O	13:AM:12:HIS:ND1	2.45	0.49
22:BA:172:A:H2'	22:BA:173:A:C8	2.47	0.49
22:BA:2331:G:P	44:BW:44:LYS:NZ	2.85	0.49
55:B8:3:G:H4'	55:B8:4:U:OP1	2.12	0.49
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.44	0.49
10:AJ:8:ILE:HG22	10:AJ:100:ILE:HA	1.94	0.49
22:BA:910:A:H2'	22:BA:911:A:C8	2.47	0.49
22:BA:2108:A:H2	22:BA:2181:U:H3	1.56	0.49
25:BD:181:ASP:HB3	25:BD:186:LEU:HB2	1.95	0.49
31:BJ:26:GLY:O	31:BJ:30:THR:HG23	2.12	0.49
56:B9:30:LYS:HE2	56:B9:63:LEU:HD23	1.93	0.49
22:BA:285:G:H2'	22:BA:286:U:C6	2.48	0.49
22:BA:286:U:H2'	22:BA:287:G:H8	1.77	0.49
22:BA:1095:A:H2'	22:BA:1096:A:C8	2.47	0.49
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.47	0.49
29:BH:129:GLU:HG3	29:BH:143:ILE:HD12	1.95	0.49
1:AA:102:G:C4	1:AA:103:U:C6	3.01	0.49
1:AA:1038:C:H2'	1:AA:1039:G:C8	2.46	0.49
3:AC:154:SER:HB3	3:AC:165:THR:HG23	1.95	0.49
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.93	0.49
10:AJ:59:LYS:HE2	10:AJ:62:ARG:NH2	2.26	0.49
27:BF:105:THR:HA	30:BI:38:SER:HB3	1.93	0.49
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.45	0.49
55:B8:23:C:H2'	55:B8:24:G:C8	2.46	0.49
1:AA:66:A:N1	1:AA:67:C:C4	2.81	0.49
1:AA:122:G:OP2	1:AA:122:G:H8	1.94	0.49
2:AB:68:LEU:HD13	2:AB:158:PRO:HG3	1.94	0.49
13:AM:16:VAL:HB	13:AM:41:GLU:HG2	1.94	0.49
22:BA:480:A:OP2	42:BU:44:LYS:HE2	2.12	0.49
22:BA:1102:C:H2'	22:BA:1103:A:C8	2.44	0.49
22:BA:1545:A:H2'	22:BA:1546:G:O4'	2.12	0.49
22:BA:2141:G:O2'	22:BA:2142:A:H5'	2.13	0.49
31:BJ:31:GLU:HG2	31:BJ:142:ILE:HG13	1.93	0.49
1:AA:344:A:H5"	1:AA:345:C:H5	1.77	0.49
1:AA:695:A:H2'	1:AA:696:A:C8	2.47	0.49
1:AA:744:C:H2'	1:AA:745:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:634:C:H2'	22:BA:635:C:H6	1.76	0.49
29:BH:121:VAL:O	29:BH:121:VAL:HG12	2.12	0.49
49:B1:35:GLU:OE2	49:B1:48:ILE:HD12	2.13	0.49
1:AA:86:G:H1'	1:AA:87:C:C5	2.47	0.49
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.77	0.49
3:AC:179:ARG:NH1	3:AC:206:GLU:OE1	2.46	0.49
16:AP:57:ILE:HG21	16:AP:75:ILE:HD11	1.95	0.49
22:BA:281:C:H2'	22:BA:282:A:H8	1.78	0.49
22:BA:1676:A:H1'	25:BD:133:THR:HG21	1.95	0.49
23:BB:29:A:H2'	23:BB:30:C:C6	2.48	0.49
1:AA:1129:C:H5"	9:AI:18:ARG:NH2	2.27	0.49
22:BA:2126:A:HO2'	22:BA:2162:G:H1	1.59	0.49
39:BR:15:SER:OG	39:BR:16:GLU:N	2.45	0.49
41:BT:92:ASN:OD1	41:BT:93:LEU:N	2.46	0.49
44:BW:71:VAL:HG22	44:BW:78:LYS:HD2	1.93	0.49
51:B3:29:LEU:HD11	51:B3:44:LEU:HB2	1.94	0.49
56:B9:104:ASP:O	56:B9:108:GLU:HG2	2.12	0.49
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.47	0.49
22:BA:2116:G:O6	22:BA:2171:A:N6	2.45	0.49
27:BF:80:ARG:H	27:BF:83:TYR:HD2	1.60	0.49
3:AC:56:VAL:CG2	3:AC:67:THR:HB	2.43	0.48
6:AF:51:ILE:HD11	6:AF:85:ILE:HD12	1.95	0.48
8:AH:10:MET:HB2	8:AH:27:MET:HE1	1.95	0.48
22:BA:1028:A:N6	22:BA:1125:G:H2'	2.28	0.48
22:BA:2639:A:H2'	22:BA:2640:G:O4'	2.11	0.48
33:BL:62:PRO:HG2	51:B3:25:LYS:HD3	1.94	0.48
41:BT:88:LYS:HB2	41:BT:91:GLN:OE1	2.12	0.48
1:AA:100:G:N2	1:AA:152:A:O2'	2.46	0.48
1:AA:1142:G:H2'	1:AA:1143:G:O4'	2.12	0.48
1:AA:1355:G:H2'	1:AA:1356:G:H8	1.78	0.48
9:AI:84:THR:HG23	9:AI:98:LEU:HD22	1.94	0.48
22:BA:645:C:H2'	22:BA:647:G:N7	2.28	0.48
22:BA:2646:C:OP2	22:BA:2732:G:O2'	2.31	0.48
25:BD:152:PRO:HG3	25:BD:156:PHE:CZ	2.48	0.48
27:BF:111:ILE:HB	27:BF:114:PHE:HB2	1.95	0.48
27:BF:162:SER:OG	27:BF:165:GLU:OE1	2.25	0.48
56:B9:7:VAL:HG23	56:B9:8:ASN:N	2.29	0.48
1:AA:451:A:H61	1:AA:481:G:H5'	1.78	0.48
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.48	0.48
8:AH:79:SER:HB2	8:AH:85:ILE:H	1.78	0.48
14:AN:32:ASP:O	14:AN:41:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:652:U:OP1	22:BA:654:A:N6	2.45	0.48
22:BA:1392:A:H5'	22:BA:1392:A:C8	2.48	0.48
22:BA:2106:U:H2'	22:BA:2107:G:C8	2.49	0.48
1:AA:56:U:H2'	1:AA:57:G:C8	2.49	0.48
1:AA:299:G:H2'	1:AA:300:A:C8	2.48	0.48
1:AA:628:G:H2'	1:AA:629:A:C8	2.48	0.48
1:AA:1036:A:H2'	1:AA:1037:C:C6	2.49	0.48
5:AE:83:HIS:CE1	5:AE:147:MET:HG3	2.48	0.48
22:BA:5:A:H2'	22:BA:6:A:C8	2.48	0.48
22:BA:608:A:H2'	22:BA:609:A:C8	2.48	0.48
24:BC:41:GLY:O	24:BC:43:ARG:NH1	2.47	0.48
1:AA:216:U:H2'	1:AA:217:C:C6	2.48	0.48
1:AA:308:C:H2'	1:AA:309:A:H8	1.79	0.48
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.48	0.48
2:AB:133:GLU:O	2:AB:137:ARG:HG2	2.13	0.48
7:AG:36:LYS:HG3	9:AI:41:ARG:HH22	1.79	0.48
13:AM:83:LEU:HD21	19:AS:74:PHE:HE1	1.79	0.48
28:BG:10:VAL:HA	28:BG:49:THR:HG22	1.94	0.48
33:BL:141:LYS:NZ	33:BL:143:GLU:OE2	2.46	0.48
41:BT:54:GLU:HG3	41:BT:88:LYS:HG3	1.94	0.48
55:B8:23:C:H2'	55:B8:24:G:H8	1.76	0.48
1:AA:100:G:H21	1:AA:152:A:H4'	1.78	0.48
1:AA:745:G:H2'	1:AA:746:A:C8	2.48	0.48
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.48	0.48
9:AI:28:ILE:HG12	9:AI:63:LEU:HD12	1.94	0.48
22:BA:959:A:H2'	22:BA:960:A:C8	2.48	0.48
22:BA:1428:C:C5	22:BA:1569:A:H5"	2.48	0.48
22:BA:2111:U:H5"	22:BA:2145:C:N3	2.29	0.48
24:BC:251:GLN:NE2	24:BC:252:THR:O	2.46	0.48
30:BI:44:PHE:CD2	30:BI:45:THR:HG23	2.48	0.48
1:AA:996:A:H2'	1:AA:997:U:C6	2.48	0.48
1:AA:1129:C:H5"	9:AI:18:ARG:HH22	1.78	0.48
3:AC:150:LYS:HG3	3:AC:201:TRP:CE3	2.48	0.48
29:BH:96:THR:HG22	29:BH:112:LYS:HA	1.94	0.48
55:B8:19:G:H4'	55:B8:20:U:OP2	2.13	0.48
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.95	0.48
6:AF:67:PRO:HB2	6:AF:69:GLU:OE1	2.14	0.48
10:AJ:87:LEU:HA	10:AJ:90:LEU:HD23	1.95	0.48
24:BC:36:LYS:NZ	24:BC:38:SER:OG	2.47	0.48
56:B9:238:ASP:HA	56:B9:266:ILE:HD12	1.96	0.48
56:B9:265:HIS:CE1	56:B9:268:THR:HG1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:808:C:OP2	15:AO:48:LYS:NZ	2.39	0.48
1:AA:1366:C:H2'	1:AA:1367:C:H6	1.79	0.48
22:BA:657:U:H2'	22:BA:658:U:C6	2.49	0.48
22:BA:1178:C:H2'	22:BA:1179:G:C8	2.47	0.48
1:AA:1297:G:H21	7:AG:114:LYS:HB3	1.79	0.48
22:BA:2314:A:H2'	22:BA:2315:G:C8	2.48	0.48
42:BU:51:ALA:O	42:BU:52:LEU:HD23	2.14	0.48
22:BA:541:A:C6	22:BA:553:G:C6	3.02	0.47
22:BA:2176:A:H2'	22:BA:2177:C:C6	2.49	0.47
24:BC:3:VAL:HG12	24:BC:19:VAL:HG22	1.96	0.47
42:BU:10:GLU:OE1	42:BU:73:PHE:HB3	2.14	0.47
56:B9:155:TRP:CD1	56:B9:353:LEU:HB2	2.48	0.47
1:AA:150:U:H2'	1:AA:151:A:H8	1.78	0.47
1:AA:1090:U:H2'	1:AA:1091:U:C6	2.49	0.47
13:AM:33:ILE:HD13	13:AM:60:VAL:HG22	1.96	0.47
22:BA:3:U:H2'	22:BA:4:U:C6	2.49	0.47
22:BA:1028:A:H2'	22:BA:1029:A:C8	2.49	0.47
22:BA:2680:U:O2'	22:BA:2681:C:H5'	2.13	0.47
26:BE:21:ARG:HH11	26:BE:106:LYS:HD2	1.79	0.47
56:B9:107:GLU:O	56:B9:111:ALA:N	2.31	0.47
1:AA:696:A:H2'	1:AA:697:U:H6	1.80	0.47
13:AM:64:VAL:O	13:AM:64:VAL:HG13	2.14	0.47
18:AR:70:TYR:HB2	18:AR:74:HIS:NE2	2.30	0.47
22:BA:357:C:H2'	22:BA:358:U:C6	2.49	0.47
22:BA:549:G:HO2'	22:BA:550:C:H6	1.60	0.47
22:BA:1932:A:H2'	22:BA:1933:G:O4'	2.14	0.47
22:BA:2182:U:H2'	22:BA:2183:A:C8	2.49	0.47
22:BA:2795:C:H2'	22:BA:2796:U:C6	2.49	0.47
40:BS:23:LEU:O	40:BS:27:LYS:NZ	2.47	0.47
1:AA:977:A:O2'	1:AA:979:C:OP2	2.31	0.47
21:AU:7:ARG:HB2	21:AU:10:GLU:OE2	2.14	0.47
22:BA:279:A:O5'	22:BA:279:A:H8	1.96	0.47
22:BA:1132:U:H3'	22:BA:1133:A:H5"	1.94	0.47
22:BA:2032:G:C5	25:BD:150:MEQ:HE3	2.49	0.47
22:BA:2387:U:H4'	44:BW:41:ARG:HH12	1.78	0.47
22:BA:2756:U:OP2	52:B4:19:ARG:NE	2.38	0.47
29:BH:44:ILE:HG13	29:BH:48:GLU:HB3	1.96	0.47
32:BK:38:ILE:HD11	32:BK:112:PHE:HZ	1.79	0.47
44:BW:32:LEU:HA	44:BW:64:ASP:OD1	2.14	0.47
54:B7:8:G:N1	56:B9:140:GLU:OE1	2.41	0.47
56:B9:17:ARG:O	56:B9:20:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:300:A:O5'	1:AA:300:A:H8	1.97	0.47
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.96	0.47
3:AC:85:GLU:OE1	3:AC:88:ARG:NH2	2.45	0.47
22:BA:851:C:OP1	47:BZ:19:LYS:HE3	2.15	0.47
28:BG:76:VAL:HA	28:BG:79:VAL:HG22	1.96	0.47
1:AA:100:G:O6	1:AA:102:G:N1	2.46	0.47
1:AA:1039:G:H2'	1:AA:1040:U:H6	1.79	0.47
3:AC:110:GLU:O	3:AC:111:LEU:HD23	2.14	0.47
3:AC:118:ASP:OD1	3:AC:119:SER:N	2.48	0.47
22:BA:1328:A:H2'	22:BA:1330:C:C5	2.50	0.47
22:BA:2261:C:C5	44:BW:16:SER:HB3	2.49	0.47
1:AA:1187:G:H2'	1:AA:1188:A:C8	2.50	0.47
2:AB:223:GLU:N	2:AB:223:GLU:OE1	2.47	0.47
3:AC:21:THR:HB	3:AC:58:GLU:OE1	2.15	0.47
3:AC:22:TRP:HB3	3:AC:59:ARG:HB2	1.96	0.47
8:AH:55:THR:O	8:AH:56:LYS:HE2	2.14	0.47
10:AJ:29:ALA:O	10:AJ:32:THR:OG1	2.27	0.47
22:BA:477:A:H2'	22:BA:478:A:C8	2.49	0.47
22:BA:632:A:H2'	22:BA:633:A:C8	2.50	0.47
22:BA:898:C:H2'	22:BA:899:A:O4'	2.15	0.47
22:BA:1078:U:H1'	22:BA:1088:A:H5'	1.97	0.47
22:BA:1433:A:H2'	22:BA:1434:A:O4'	2.14	0.47
22:BA:1747:U:H2'	22:BA:1748:C:C6	2.49	0.47
22:BA:2100:G:C6	22:BA:2190:G:C5	3.03	0.47
22:BA:2130:U:H2'	22:BA:2158:A:C6	2.50	0.47
22:BA:2172:U:OP2	22:BA:2173:A:H5"	2.15	0.47
22:BA:2577:A:H5"	22:BA:2578:G:H5'	1.96	0.47
22:BA:2845:U:H5"	37:BP:52:ASN:O	2.14	0.47
44:BW:25:ARG:HD3	44:BW:31:VAL:HG12	1.95	0.47
50:B2:31:LEU:HD22	50:B2:42:LEU:HD23	1.97	0.47
56:B9:69:THR:O	56:B9:73:MET:HG2	2.15	0.47
56:B9:144:TRP:CE3	56:B9:201:LEU:HD22	2.49	0.47
1:AA:390:U:H2'	1:AA:391:G:H8	1.80	0.47
1:AA:1071:C:H2'	1:AA:1072:G:C8	2.50	0.47
2:AB:196:VAL:HG23	2:AB:199:VAL:HG22	1.96	0.47
22:BA:876:C:H2'	22:BA:877:A:O4'	2.15	0.47
22:BA:967:U:H2'	22:BA:968:C:C6	2.50	0.47
22:BA:1182:G:H2'	22:BA:1183:U:O4'	2.14	0.47
25:BD:16:THR:OG1	25:BD:18:ASP:OD1	2.25	0.47
51:B3:15:LYS:HB2	51:B3:23:LYS:HE3	1.95	0.47
9:AI:118:LEU:HD22	9:AI:124:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:94:GLU:O	11:AK:97:ILE:HG22	2.14	0.47
22:BA:2640:G:P	31:BJ:96:ARG:HH11	2.38	0.47
29:BH:103:VAL:O	29:BH:107:GLY:N	2.36	0.47
1:AA:185:U:H2'	1:AA:186:C:C6	2.50	0.47
17:AQ:21:ILE:HG12	17:AQ:48:ASP:HB2	1.97	0.47
22:BA:1466:U:O2'	22:BA:1546:G:O2'	2.17	0.47
25:BD:1:MET:SD	25:BD:2:ILE:N	2.88	0.47
1:AA:100:G:O2'	1:AA:102:G:C5'	2.62	0.46
1:AA:674:G:H2'	1:AA:675:A:C8	2.50	0.46
4:AD:184:ARG:NH1	4:AD:187:GLU:OE1	2.48	0.46
6:AF:12:PRO:O	6:AF:15:SER:OG	2.22	0.46
9:AI:52:LEU:HD11	9:AI:63:LEU:HD11	1.97	0.46
9:AI:67:VAL:HG21	9:AI:79:ILE:HD11	1.97	0.46
22:BA:1038:G:H2'	22:BA:1039:A:C8	2.50	0.46
22:BA:1114:C:O2'	22:BA:1115:G:H5'	2.16	0.46
24:BC:144:VAL:HB	24:BC:154:LEU:HB2	1.97	0.46
56:B9:294:LYS:HE3	56:B9:294:LYS:HB2	1.83	0.46
1:AA:68:G:H5'	1:AA:171:A:C1'	2.45	0.46
1:AA:505:G:H2'	1:AA:506:G:H8	1.80	0.46
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.51	0.46
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.75	0.46
6:AF:4:TYR:CE2	6:AF:71:ILE:HG13	2.50	0.46
6:AF:101:PRO:HA	6:AF:104:LYS:HG2	1.95	0.46
14:AN:20:PHE:C	14:AN:22:LYS:H	2.19	0.46
22:BA:1889:A:H2'	22:BA:1890:A:C8	2.50	0.46
1:AA:208:U:H3'	1:AA:210:C:H41	1.79	0.46
1:AA:591:U:H2'	1:AA:592:G:H8	1.80	0.46
1:AA:718:A:H5'	11:AK:119:ASN:ND2	2.30	0.46
16:AP:47:GLU:N	16:AP:47:GLU:OE1	2.48	0.46
22:BA:299:A:H2'	22:BA:300:A:C8	2.50	0.46
22:BA:414:C:H2'	22:BA:415:A:H8	1.81	0.46
22:BA:1724:G:H2'	22:BA:1725:U:C6	2.50	0.46
1:AA:362:G:N2	1:AA:365:U:OP2	2.44	0.46
1:AA:1268:G:H2'	1:AA:1269:A:C8	2.50	0.46
2:AB:204:ASP:OD1	2:AB:205:ASP:N	2.48	0.46
3:AC:58:GLU:HB2	3:AC:65:ARG:HG2	1.97	0.46
4:AD:104:ARG:HH21	4:AD:111:ARG:HH12	1.64	0.46
5:AE:13:GLU:HG3	5:AE:39:VAL:HG23	1.97	0.46
14:AN:83:LYS:HA	14:AN:83:LYS:HD3	1.73	0.46
22:BA:1174:U:H2'	22:BA:1175:A:C8	2.50	0.46
1:AA:72:A:C5	1:AA:73:C:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:100:G:C2	1:AA:102:G:C4	3.04	0.46
9:AI:25:ASN:OD1	9:AI:27:LYS:NZ	2.39	0.46
17:AQ:46:VAL:HG11	17:AQ:61:ILE:HD12	1.98	0.46
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.50	0.46
22:BA:2557:G:H2'	22:BA:2558:C:C6	2.50	0.46
34:BM:58:LYS:O	34:BM:59:ARG:HG3	2.16	0.46
42:BU:62:GLU:OE1	42:BU:62:GLU:N	2.48	0.46
1:AA:100:G:C4	1:AA:102:G:N9	2.82	0.46
1:AA:834:U:H2'	1:AA:835:U:C6	2.50	0.46
10:AJ:32:THR:HB	10:AJ:83:THR:HG22	1.96	0.46
22:BA:1171:G:H3'	22:BA:1173:U:O4	2.15	0.46
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.48	0.46
22:BA:2101:A:C2	22:BA:2189:U:O2	2.69	0.46
22:BA:2271:G:OP1	44:BW:18:ALA:HB1	2.16	0.46
22:BA:2803:G:H2'	22:BA:2804:U:C6	2.51	0.46
56:B9:93:GLU:HA	56:B9:96:PHE:HB3	1.97	0.46
1:AA:177:G:OP1	20:AT:60:ARG:HD2	2.15	0.46
1:AA:486:U:H2'	1:AA:487:A:C8	2.51	0.46
5:AE:112:ARG:O	5:AE:116:GLU:HG3	2.16	0.46
22:BA:1065:U:H2'	22:BA:1066:U:C6	2.51	0.46
22:BA:2595:G:N2	22:BA:2598:A:OP2	2.35	0.46
42:BU:101:GLU:OE1	42:BU:101:GLU:N	2.47	0.46
1:AA:954:G:H2'	1:AA:955:U:C6	2.50	0.46
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.16	0.46
22:BA:883:G:H2'	22:BA:883:G:N3	2.31	0.46
27:BF:10:ASP:HB2	27:BF:11:GLU:OE1	2.15	0.46
30:BI:59:ARG:HH22	30:BI:63:ARG:HH22	1.64	0.46
56:B9:95:THR:HA	56:B9:98:GLU:HB2	1.97	0.46
1:AA:64:G:H21	1:AA:69:G:H3'	1.81	0.46
1:AA:67:C:C4	1:AA:69:G:N3	2.84	0.46
1:AA:100:G:C8	1:AA:102:G:N7	2.84	0.46
1:AA:434:U:H2'	1:AA:435:A:C8	2.50	0.46
1:AA:466:A:N3	1:AA:467:U:H5	2.13	0.46
1:AA:539:A:H2'	1:AA:540:G:H8	1.80	0.46
10:AJ:55:PRO:HA	14:AN:82:ILE:HD11	1.98	0.46
22:BA:2314:A:H2'	22:BA:2315:G:H8	1.80	0.46
23:BB:2:G:H2'	23:BB:3:C:C6	2.51	0.46
29:BH:110:VAL:HG21	29:BH:132:PHE:HE2	1.81	0.46
39:BR:43:ASN:O	39:BR:46:GLU:HG3	2.16	0.46
1:AA:1014:A:C2	1:AA:1219:A:H1'	2.51	0.46
1:AA:1121:U:C2	1:AA:1122:U:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:613:A:H5”	22:BA:614:A:C8	2.51	0.46
26:BE:121:VAL:O	26:BE:190:ALA:N	2.49	0.46
27:BF:11:GLU:OE1	27:BF:11:GLU:N	2.49	0.46
42:BU:41:LEU:HA	42:BU:62:GLU:HA	1.98	0.46
42:BU:85:PHE:CE1	42:BU:94:ARG:HG2	2.51	0.46
1:AA:45:G:H2’	1:AA:46:G:H8	1.82	0.45
1:AA:76:G:C6	1:AA:77:A:C5	3.04	0.45
1:AA:408:A:O3’	4:AD:23:SER:OG	2.34	0.45
1:AA:575:G:O2’	1:AA:821:G:OP2	2.21	0.45
1:AA:1377:A:OP1	7:AG:92:ARG:NH2	2.49	0.45
3:AC:155:GLY:O	3:AC:196:ILE:HG12	2.16	0.45
6:AF:35:LYS:HB2	6:AF:65:GLU:HB2	1.97	0.45
19:AS:6:LYS:HZ2	30:BI:63:ARG:HD3	1.82	0.45
21:AU:11:PRO:HG2	21:AU:14:VAL:HG13	1.98	0.45
22:BA:250:G:H2’	22:BA:251:A:C8	2.51	0.45
22:BA:644:A:H2’	22:BA:645:C:O4’	2.16	0.45
22:BA:667:U:H2’	22:BA:668:A:O4’	2.15	0.45
22:BA:1067:A:O2’	22:BA:1068:G:O4’	2.34	0.45
23:BB:2:G:H2’	23:BB:3:C:H6	1.81	0.45
1:AA:210:C:H1’	1:AA:211:G:N2	2.30	0.45
1:AA:1086:U:H3	1:AA:1099:G:H22	1.64	0.45
22:BA:1079:C:H2’	22:BA:1080:A:H8	1.81	0.45
22:BA:2812:G:H2’	22:BA:2813:A:C8	2.51	0.45
24:BC:21:ASN:HB3	24:BC:24:LEU:HD13	1.98	0.45
40:BS:59:GLU:HG2	40:BS:60:HIS:N	2.30	0.45
47:BZ:13:ALA:O	47:BZ:21:LYS:HE2	2.16	0.45
49:B1:40:ASP:HB3	49:B1:43:VAL:HG12	1.98	0.45
56:B9:27:TYR:CE1	56:B9:67:VAL:HA	2.51	0.45
1:AA:64:G:N2	1:AA:70:U:C5	2.84	0.45
1:AA:100:G:C2	1:AA:102:G:H1’	2.50	0.45
1:AA:1042:A:O2’	1:AA:1043:G:O5’	2.32	0.45
1:AA:1316:G:H22	1:AA:1318:A:H3’	1.81	0.45
14:AN:90:ARG:HB2	14:AN:92:GLU:OE1	2.17	0.45
22:BA:645:C:H2’	22:BA:647:G:C8	2.52	0.45
22:BA:1201:U:H2’	22:BA:1202:G:H8	1.81	0.45
22:BA:1434:A:H2’	22:BA:1435:G:C8	2.51	0.45
25:BD:108:ASP:OD1	25:BD:173:GLN:HA	2.16	0.45
26:BE:153:LEU:HB2	26:BE:171:ASP:OD2	2.16	0.45
27:BF:8:TYR:O	27:BF:13:VAL:HG13	2.15	0.45
1:AA:1149:C:H2’	1:AA:1150:A:C8	2.51	0.45
1:AA:1305:G:N2	1:AA:1332:A:H2	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2064:C:H2'	22:BA:2065:C:C6	2.51	0.45
29:BH:86:ASP:OD1	29:BH:87:GLU:N	2.45	0.45
1:AA:64:G:C4	1:AA:69:G:C5	3.05	0.45
1:AA:958:A:C6	19:AS:55:ARG:HG2	2.52	0.45
1:AA:1309:G:N7	13:AM:98:ARG:NH2	2.63	0.45
13:AM:71:ARG:NH2	27:BF:113:ASP:OD2	2.50	0.45
22:BA:884:U:H1'	22:BA:893:C:C2	2.52	0.45
22:BA:899:A:HO2'	22:BA:900:A:H8	1.63	0.45
22:BA:948:C:H1'	22:BA:984:A:C8	2.51	0.45
40:BS:73:LYS:HB3	40:BS:106:VAL:HB	1.98	0.45
42:BU:48:PRO:HB3	42:BU:56:GLY:H	1.81	0.45
50:B2:44:VAL:HG23	50:B2:44:VAL:O	2.17	0.45
56:B9:49:GLU:OE1	56:B9:52:ARG:NH2	2.49	0.45
1:AA:390:U:H2'	1:AA:391:G:C8	2.50	0.45
1:AA:633:G:H2'	1:AA:634:C:C6	2.51	0.45
10:AJ:10:LEU:HD23	10:AJ:98:VAL:HG12	1.98	0.45
13:AM:46:SER:OG	13:AM:47:GLU:N	2.50	0.45
22:BA:1816:C:N4	24:BC:35:GLU:OE1	2.47	0.45
22:BA:2130:U:H5"	22:BA:2133:G:OP1	2.17	0.45
41:BT:48:GLN:HE21	41:BT:55:VAL:H	1.65	0.45
56:B9:338:THR:OG1	56:B9:339:GLY:HA2	2.16	0.45
1:AA:473:U:H2'	1:AA:474:G:C8	2.50	0.45
1:AA:891:U:H2'	1:AA:892:A:H8	1.81	0.45
1:AA:1170:A:H2'	1:AA:1171:A:O4'	2.15	0.45
1:AA:1202:U:N3	14:AN:82:ILE:HG21	2.32	0.45
4:AD:117:LEU:HD23	4:AD:117:LEU:HA	1.76	0.45
9:AI:25:ASN:H	9:AI:27:LYS:HZ3	1.62	0.45
19:AS:5:LEU:HD13	19:AS:5:LEU:HA	1.74	0.45
22:BA:1425:G:H2'	22:BA:1426:G:C8	2.51	0.45
22:BA:1689:A:H2'	22:BA:1690:A:C8	2.52	0.45
22:BA:2183:A:H2'	22:BA:2184:A:C8	2.52	0.45
22:BA:2640:G:P	31:BJ:96:ARG:NH1	2.90	0.45
31:BJ:110:PRO:O	31:BJ:115:GLY:HA3	2.17	0.45
40:BS:35:ILE:O	40:BS:39:THR:HG23	2.17	0.45
52:B4:18:LYS:HE3	52:B4:21:GLY:HA2	1.98	0.45
56:B9:40:GLU:O	56:B9:43:GLN:HG2	2.16	0.45
1:AA:100:G:C4	1:AA:102:G:C4	3.05	0.45
1:AA:193:C:H2'	1:AA:194:C:H6	1.81	0.45
1:AA:946:A:H2'	1:AA:947:G:C8	2.51	0.45
1:AA:1009:U:H3	1:AA:1020:G:H1	1.65	0.45
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.17	0.45
22:BA:1096:A:C2	22:BA:1097:U:H1'	2.52	0.45
22:BA:2100:G:H3'	22:BA:2101:A:C8	2.51	0.45
22:BA:2130:U:H4'	22:BA:2133:G:H4'	1.97	0.45
22:BA:2315:G:H2'	22:BA:2316:G:H8	1.82	0.45
24:BC:176:LEU:HD12	24:BC:180:GLU:OE1	2.16	0.45
42:BU:99:ASN:OD1	42:BU:99:ASN:N	2.50	0.45
56:B9:61:SER:HA	56:B9:64:GLU:HG3	1.99	0.45
56:B9:280:GLN:O	56:B9:284:LYS:N	2.37	0.45
1:AA:494:G:H2'	1:AA:496:A:H8	1.82	0.45
1:AA:1129:C:H4'	9:AI:18:ARG:HH22	1.81	0.45
2:AB:210:VAL:HA	2:AB:213:TYR:CD2	2.51	0.45
10:AJ:7:ARG:HG3	10:AJ:73:LEU:HD11	1.99	0.45
20:AT:43:ASP:OD1	20:AT:44:LYS:N	2.50	0.45
22:BA:359:G:C6	22:BA:360:U:C4	3.05	0.45
22:BA:2107:G:O6	22:BA:2183:A:N6	2.50	0.45
22:BA:2591:C:H2'	22:BA:2592:G:C8	2.51	0.45
27:BF:12:VAL:HA	27:BF:15:LYS:HG2	1.99	0.45
1:AA:308:C:H2'	1:AA:309:A:C8	2.52	0.45
22:BA:832:U:H2'	22:BA:833:A:C8	2.52	0.45
22:BA:2330:G:O3'	44:BW:44:LYS:NZ	2.44	0.45
25:BD:114:LYS:HE2	25:BD:196:ALA:HB2	1.98	0.45
55:B8:69:A:H2'	55:B8:70:C:C6	2.52	0.45
1:AA:67:C:O2	1:AA:171:A:H2	2.00	0.44
1:AA:723:U:O4	21:AU:53:VAL:HG22	2.17	0.44
1:AA:954:G:H21	1:AA:1227:A:H62	1.65	0.44
1:AA:1120:C:C2	1:AA:1121:U:C5	3.05	0.44
1:AA:1230:C:H5'	55:B8:30:C:H5"	1.99	0.44
3:AC:152:GLU:HG3	3:AC:167:TRP:HB3	1.98	0.44
18:AR:21:ILE:HG21	18:AR:55:LEU:HD23	1.99	0.44
34:BM:81:4D4:H14	34:BM:81:4D4:H10	1.60	0.44
1:AA:6:G:O2'	1:AA:298:A:H1'	2.17	0.44
1:AA:235:C:H2'	1:AA:236:A:H8	1.81	0.44
12:AL:107:VAL:HG23	12:AL:110:ARG:HB2	2.00	0.44
22:BA:359:G:C5	22:BA:360:U:C4	3.05	0.44
22:BA:952:G:C6	22:BA:966:G:C6	3.04	0.44
22:BA:1052:C:H2'	22:BA:1053:C:H6	1.81	0.44
22:BA:1357:C:H2'	22:BA:1358:G:O4'	2.17	0.44
22:BA:1632:A:H2'	22:BA:1633:G:C8	2.51	0.44
22:BA:2312:U:H5'	27:BF:85:ILE:HD11	1.98	0.44
26:BE:118:LEU:HD11	26:BE:188:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B0:13:ARG:O	48:B0:17:ARG:HG3	2.16	0.44
56:B9:277:ASP:O	56:B9:283:ASN:ND2	2.47	0.44
1:AA:440:C:C2	1:AA:441:A:C8	3.05	0.44
1:AA:883:C:O2'	1:AA:884:U:H5'	2.18	0.44
22:BA:277:G:O2'	22:BA:361:G:O6	2.33	0.44
22:BA:1809:A:O5'	22:BA:1809:A:H8	2.01	0.44
29:BH:70:GLU:O	29:BH:71:LYS:HB3	2.18	0.44
29:BH:108:VAL:HG23	29:BH:109:GLU:HG3	1.99	0.44
41:BT:68:LYS:O	41:BT:74:ILE:HD12	2.17	0.44
1:AA:459:A:N1	1:AA:460:A:C6	2.85	0.44
1:AA:718:A:H2	18:AR:38:LYS:HE2	1.81	0.44
1:AA:908:A:H2'	1:AA:909:A:H8	1.82	0.44
1:AA:1118:U:OP1	9:AI:11:ARG:NH1	2.43	0.44
2:AB:27:MET:HE3	2:AB:193:PRO:HD3	2.00	0.44
2:AB:60:ILE:HA	2:AB:63:ARG:HH12	1.82	0.44
7:AG:115:SER:O	7:AG:119:ARG:HB2	2.17	0.44
22:BA:274:C:C5	22:BA:275:C:N3	2.85	0.44
22:BA:541:A:N1	22:BA:553:G:C6	2.85	0.44
22:BA:1076:C:H2'	22:BA:1077:A:C8	2.52	0.44
22:BA:1079:C:H2'	22:BA:1080:A:C8	2.53	0.44
22:BA:1282:U:H2'	22:BA:1283:G:O4'	2.17	0.44
1:AA:751:U:H2'	1:AA:752:G:O4'	2.17	0.44
2:AB:192:ASP:OD1	2:AB:192:ASP:N	2.51	0.44
6:AF:38:ARG:NE	6:AF:63:ASN:OD1	2.49	0.44
9:AI:98:LEU:HD23	9:AI:103:PHE:HD2	1.82	0.44
22:BA:848:C:H2'	22:BA:849:A:H8	1.82	0.44
22:BA:1077:A:H2	22:BA:1088:A:HO2'	1.66	0.44
22:BA:1505:A:H2'	22:BA:1506:U:O4'	2.17	0.44
22:BA:2724:U:H2'	22:BA:2725:A:C8	2.53	0.44
25:BD:36:GLN:HB3	25:BD:49:GLN:HE21	1.83	0.44
28:BG:149:ARG:HA	28:BG:162:VAL:HG13	1.99	0.44
42:BU:48:PRO:HB3	42:BU:56:GLY:N	2.32	0.44
1:AA:198:G:H2'	1:AA:199:A:H8	1.83	0.44
1:AA:868:C:H2'	1:AA:869:G:O4'	2.17	0.44
1:AA:1181:G:O2'	1:AA:1182:G:N7	2.48	0.44
1:AA:1318:A:H1'	19:AS:37:ARG:NH1	2.32	0.44
22:BA:372:G:C8	45:BX:61:LYS:HD2	2.52	0.44
22:BA:1085:A:C8	22:BA:1086:A:C6	3.05	0.44
22:BA:1729:U:C2	22:BA:1731:G:N2	2.84	0.44
22:BA:2123:G:C6	22:BA:2176:A:N6	2.86	0.44
29:BH:134:VAL:HG23	29:BH:138:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BN:16:HIS:O	35:BN:16:HIS:CD2	2.70	0.44
1:AA:113:G:H1'	1:AA:354:G:H5'	1.99	0.44
1:AA:1014:A:H2'	1:AA:1015:G:C8	2.53	0.44
1:AA:1040:U:H2'	1:AA:1041:G:H8	1.83	0.44
1:AA:1171:A:H2'	1:AA:1172:C:H6	1.83	0.44
1:AA:1308:U:OP2	13:AM:100:GLN:NE2	2.49	0.44
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.53	0.44
7:AG:113:ASP:OD2	7:AG:122:ASN:ND2	2.47	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HD11	2.00	0.44
11:AK:37:ARG:NH1	11:AK:83:GLU:OE2	2.51	0.44
17:AQ:77:ARG:NH1	17:AQ:79:VAL:HG12	2.33	0.44
22:BA:856:G:H2'	22:BA:857:G:C8	2.53	0.44
22:BA:2038:G:H2'	22:BA:2039:U:O4'	2.17	0.44
22:BA:2522:U:O2'	22:BA:2647:U:OP1	2.27	0.44
37:BP:6:LYS:O	37:BP:10:GLN:HG2	2.17	0.44
51:B3:29:LEU:HD11	51:B3:44:LEU:CB	2.47	0.44
55:B8:63:U:H2'	55:B8:64:C:C6	2.53	0.44
56:B9:27:TYR:HE1	56:B9:67:VAL:HA	1.83	0.44
1:AA:131:A:H2'	1:AA:132:C:C6	2.53	0.44
1:AA:715:A:H2'	1:AA:716:A:C8	2.53	0.44
1:AA:890:G:O2'	1:AA:906:A:N6	2.51	0.44
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.53	0.44
1:AA:1120:C:H2'	1:AA:1121:U:C6	2.53	0.44
1:AA:1202:U:C2	14:AN:82:ILE:HG21	2.53	0.44
8:AH:12:THR:HG22	8:AH:15:ARG:NH1	2.19	0.44
9:AI:60:LYS:HE2	9:AI:60:LYS:HB2	1.82	0.44
22:BA:176:A:O2'	22:BA:177:G:H5'	2.18	0.44
22:BA:1733:G:H2'	22:BA:1734:G:H8	1.83	0.44
22:BA:2523:G:HO2'	22:BA:2764:A:HO2'	1.63	0.44
22:BA:2554:U:H2'	22:BA:2555:U:C6	2.52	0.44
41:BT:4:GLU:HG2	41:BT:49:LYS:HE2	1.99	0.44
49:B1:5:ILE:HG23	49:B1:28:ARG:NH1	2.32	0.44
49:B1:17:THR:HG21	49:B1:42:VAL:HG13	2.00	0.44
1:AA:1340:A:O2'	55:B8:32:U:H5'	2.18	0.44
16:AP:69:ASP:OD1	16:AP:70:ARG:N	2.51	0.44
19:AS:29:LYS:HG2	19:AS:30:PRO:HD2	2.00	0.44
22:BA:2099:U:H2'	22:BA:2100:G:O4'	2.17	0.44
22:BA:2113:U:H3'	22:BA:2115:G:N2	2.33	0.44
26:BE:48:THR:HG22	26:BE:86:ALA:HB3	1.99	0.44
27:BF:137:ILE:HG13	27:BF:138:PHE:N	2.32	0.44
29:BH:101:ASP:O	29:BH:104:THR:OG1	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BQ:48:ARG:NH1	38:BQ:49:ASP:OD1	2.51	0.44
42:BU:51:ALA:C	42:BU:53:ASN:H	2.21	0.44
1:AA:45:G:H2'	1:AA:46:G:C8	2.52	0.43
1:AA:389:A:H3'	1:AA:390:U:C6	2.53	0.43
1:AA:1010:U:H2'	1:AA:1011:C:H6	1.82	0.43
17:AQ:60:GLU:OE1	17:AQ:77:ARG:NH2	2.51	0.43
20:AT:44:LYS:NZ	20:AT:87:ALA:OXT	2.38	0.43
22:BA:1175:A:H1'	22:BA:1176:U:C6	2.53	0.43
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.83	0.43
22:BA:2181:U:H2'	22:BA:2182:U:O4'	2.18	0.43
25:BD:22:ILE:HG23	25:BD:190:LYS:HG3	2.00	0.43
36:BO:110:ALA:O	36:BO:115:LEU:HB3	2.17	0.43
1:AA:102:G:N3	1:AA:151:A:H2	2.16	0.43
1:AA:270:A:H2'	1:AA:271:C:C6	2.52	0.43
1:AA:462:G:C6	1:AA:463:U:C4	3.06	0.43
1:AA:683:G:N2	11:AK:39:GLY:O	2.51	0.43
2:AB:144:LEU:HD23	2:AB:144:LEU:O	2.18	0.43
8:AH:8:ALA:O	8:AH:12:THR:HG23	2.19	0.43
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.43
18:AR:22:ASP:OD2	18:AR:24:LYS:HE2	2.18	0.43
22:BA:810:U:C4	33:BL:29:LYS:O	2.71	0.43
22:BA:1027:A:C2	22:BA:2488:G:H5'	2.53	0.43
22:BA:2185:U:H2'	22:BA:2186:G:C8	2.53	0.43
23:BB:42:C:C6	27:BF:66:LEU:HB2	2.53	0.43
34:BM:58:LYS:C	34:BM:59:ARG:HG3	2.39	0.43
39:BR:14:VAL:HG12	39:BR:20:VAL:HG11	2.00	0.43
39:BR:44:GLY:O	39:BR:45:GLU:HG2	2.16	0.43
43:BV:26:PHE:HE2	43:BV:89:ILE:HG12	1.82	0.43
56:B9:31:LYS:HD2	56:B9:34:LEU:HD12	1.99	0.43
1:AA:73:C:H2'	1:AA:74:A:O4'	2.18	0.43
1:AA:149:A:H2'	1:AA:150:U:C6	2.53	0.43
1:AA:269:C:H2'	1:AA:270:A:C8	2.53	0.43
4:AD:4:TYR:CE2	4:AD:11:LEU:HD11	2.53	0.43
7:AG:113:ASP:O	7:AG:119:ARG:NH2	2.48	0.43
22:BA:45:G:H5"	22:BA:46:G:O5'	2.18	0.43
22:BA:1250:G:H5"	38:BQ:6:ARG:CD	2.44	0.43
22:BA:2193:G:H2'	22:BA:2194:U:C6	2.53	0.43
22:BA:2251:OMG:HM23	22:BA:2251:OMG:H1'	1.73	0.43
24:BC:267:ILE:HG21	24:BC:270:ARG:HD2	1.98	0.43
27:BF:14:LYS:O	27:BF:18:THR:HG23	2.17	0.43
55:B8:62:C:H2'	55:B8:63:U:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:9:ASN:O	56:B9:13:ASP:N	2.50	0.43
56:B9:33:ARG:HD2	56:B9:63:LEU:HD11	1.99	0.43
1:AA:71:A:C6	1:AA:101:A:C6	3.06	0.43
1:AA:461:A:C6	1:AA:462:G:O6	2.72	0.43
1:AA:757:U:OP1	1:AA:822:U:O2'	2.26	0.43
22:BA:839:U:H2'	22:BA:840:C:C6	2.53	0.43
22:BA:1278:C:H2'	22:BA:1279:G:C8	2.53	0.43
22:BA:2108:A:N1	22:BA:2181:U:O4	2.51	0.43
22:BA:2113:U:P	22:BA:2115:G:H1	2.42	0.43
22:BA:2298:A:N6	22:BA:2321:U:O4	2.52	0.43
1:AA:66:A:C5	1:AA:67:C:C5	3.07	0.43
1:AA:100:G:C2	1:AA:101:A:C2	3.06	0.43
1:AA:451:A:H1'	1:AA:452:A:C2	2.54	0.43
1:AA:696:A:H2'	1:AA:697:U:C6	2.54	0.43
13:AM:89:LEU:HA	13:AM:92:ARG:HG2	2.00	0.43
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.51	0.43
22:BA:161:A:OP2	22:BA:162:U:O2'	2.31	0.43
22:BA:548:G:N3	22:BA:548:G:H2'	2.33	0.43
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.54	0.43
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.83	0.43
22:BA:1720:U:H2'	22:BA:1721:G:O4'	2.17	0.43
22:BA:2265:U:OP2	22:BA:2266:A:O2'	2.36	0.43
24:BC:75:PRO:HG2	24:BC:97:LYS:HG3	2.00	0.43
1:AA:460:A:C6	1:AA:461:A:C6	3.06	0.43
1:AA:779:C:H2'	1:AA:780:A:O4'	2.18	0.43
1:AA:1048:G:H4'	14:AN:2:LYS:NZ	2.34	0.43
1:AA:1315:U:O2	1:AA:1360:A:H2	2.02	0.43
2:AB:20:THR:HG22	2:AB:39:HIS:CD2	2.54	0.43
22:BA:893:C:H2'	22:BA:894:U:O4'	2.19	0.43
22:BA:1664:A:H2	32:BK:1:MET:HE1	1.82	0.43
22:BA:2389:G:H5"	22:BA:2390:U:O4'	2.19	0.43
27:BF:73:SER:OG	27:BF:80:ARG:HA	2.19	0.43
30:BI:16:CYS:SG	30:BI:17:SER:N	2.92	0.43
56:B9:124:ASP:O	56:B9:187:TYR:HA	2.18	0.43
1:AA:67:C:N4	1:AA:69:G:C6	2.87	0.43
1:AA:162:A:O5'	1:AA:162:A:H8	1.99	0.43
1:AA:1121:U:H2'	1:AA:1122:U:H6	1.84	0.43
1:AA:1141:C:H2'	1:AA:1142:G:H8	1.83	0.43
3:AC:59:ARG:CZ	3:AC:64:ILE:HD12	2.49	0.43
13:AM:19:LEU:HD23	13:AM:19:LEU:HA	1.83	0.43
13:AM:66:GLU:HG3	13:AM:67:GLY:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:593:U:H2'	22:BA:594:U:C6	2.53	0.43
22:BA:685:A:H5"	22:BA:788:A:H62	1.84	0.43
22:BA:2700:A:H2'	22:BA:2701:U:C6	2.53	0.43
33:BL:78:ARG:HG2	33:BL:113:ALA:HB3	2.00	0.43
55:B8:51:A:H2'	55:B8:52:G:C8	2.54	0.43
1:AA:1306:A:O2'	13:AM:108:THR:HG21	2.18	0.43
21:AU:4:ILE:O	21:AU:4:ILE:HG13	2.18	0.43
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.49	0.43
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	2.00	0.43
24:BC:28:LYS:HA	24:BC:28:LYS:HD3	1.86	0.43
1:AA:445:G:N1	1:AA:489:C:H5	2.00	0.43
1:AA:1143:G:H2'	1:AA:1144:G:H8	1.84	0.43
2:AB:111:ILE:O	2:AB:114:LEU:HB3	2.19	0.43
2:AB:219:ALA:O	2:AB:221:VAL:N	2.52	0.43
22:BA:1179:G:H2'	22:BA:1180:U:C6	2.54	0.43
22:BA:2514:U:H2'	22:BA:2515:C:C6	2.53	0.43
1:AA:335:C:H2'	1:AA:336:A:C8	2.54	0.43
1:AA:457:G:H22	1:AA:474:G:N2	2.16	0.43
1:AA:466:A:O2'	1:AA:467:U:H6	2.01	0.43
1:AA:1493:A:H4'	1:AA:1494:G:OP1	2.18	0.43
19:AS:28:LYS:HE2	19:AS:28:LYS:HB2	1.89	0.43
22:BA:285:G:H2'	22:BA:286:U:H6	1.83	0.43
22:BA:422:A:O5'	22:BA:422:A:H8	2.01	0.43
22:BA:2174:C:H2'	22:BA:2175:C:C6	2.54	0.43
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.52	0.43
34:BM:70:ASP:OD1	34:BM:70:ASP:N	2.52	0.43
42:BU:49:VAL:HG22	42:BU:51:ALA:H	1.83	0.43
56:B9:338:THR:H	56:B9:339:GLY:HA2	1.83	0.43
1:AA:412:A:O2'	1:AA:414:A:H5'	2.19	0.42
1:AA:471:U:H2'	1:AA:472:U:C6	2.54	0.42
1:AA:473:U:C2	1:AA:474:G:C8	3.07	0.42
12:AL:36:ARG:HG2	12:AL:38:TYR:CD1	2.53	0.42
22:BA:2139:U:O4	22:BA:2152:G:O6	2.37	0.42
25:BD:33:ARG:HH22	25:BD:74:GLU:HG3	1.84	0.42
26:BE:191:ASP:O	26:BE:195:GLN:HG3	2.19	0.42
56:B9:21:LEU:HB2	56:B9:25:LEU:HD12	2.01	0.42
14:AN:98:LYS:HE3	14:AN:98:LYS:HB3	1.79	0.42
18:AR:38:LYS:HB2	18:AR:38:LYS:HE3	1.72	0.42
22:BA:1870:C:O2'	22:BA:1871:A:O4'	2.37	0.42
22:BA:2031:A:C6	22:BA:2498:OMC:H1'	2.54	0.42
22:BA:2537:U:H2'	22:BA:2538:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:49:C:H2'	23:BB:50:A:C8	2.54	0.42
24:BC:247:PRO:HG2	24:BC:248:TRP:CZ3	2.54	0.42
29:BH:4:ILE:HD13	29:BH:43:ASN:HB2	2.01	0.42
41:BT:18:GLU:HG2	41:BT:19:LYS:N	2.34	0.42
43:BV:72:VAL:HB	43:BV:91:PHE:HB3	2.01	0.42
1:AA:100:G:C4	1:AA:101:A:C6	3.08	0.42
5:AE:160:SER:HA	5:AE:164:ILE:HD11	2.01	0.42
7:AG:60:GLU:OE1	7:AG:60:GLU:N	2.47	0.42
10:AJ:77:VAL:HG23	10:AJ:78:GLU:OE1	2.18	0.42
11:AK:28:ASN:O	11:AK:57:LYS:HE3	2.19	0.42
22:BA:280:U:C4	22:BA:360:U:O2	2.71	0.42
22:BA:1068:G:C8	22:BA:1069:A:N7	2.88	0.42
22:BA:1175:A:C8	22:BA:1176:U:N3	2.87	0.42
22:BA:2149:U:H2'	22:BA:2150:C:C6	2.54	0.42
29:BH:4:ILE:HA	29:BH:17:ASP:O	2.19	0.42
1:AA:75:G:C5	1:AA:76:G:C8	3.07	0.42
1:AA:193:C:H2'	1:AA:194:C:C6	2.53	0.42
1:AA:264:C:H2'	1:AA:265:G:O4'	2.19	0.42
1:AA:593:U:H2'	1:AA:594:U:H6	1.85	0.42
1:AA:745:G:H2'	1:AA:746:A:H8	1.83	0.42
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.48	0.42
1:AA:983:A:H5"	1:AA:984:C:OP2	2.19	0.42
1:AA:1005:A:H3'	1:AA:1006:G:H8	1.83	0.42
1:AA:1009:U:H2'	1:AA:1010:U:C6	2.54	0.42
6:AF:101:PRO:N	6:AF:104:LYS:HE3	2.34	0.42
22:BA:1050:A:C2	22:BA:2751:G:C4	3.08	0.42
22:BA:2165:C:H2'	22:BA:2166:U:O4'	2.19	0.42
22:BA:2228:G:H2'	22:BA:2229:U:C6	2.54	0.42
1:AA:64:G:C5	1:AA:69:G:C6	3.06	0.42
1:AA:64:G:N1	1:AA:69:G:C2	2.87	0.42
1:AA:75:G:C6	1:AA:76:G:C5	3.08	0.42
1:AA:413:G:N2	1:AA:428:G:H1'	2.35	0.42
1:AA:727:G:N2	1:AA:730:G:OP2	2.43	0.42
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.37	0.42
22:BA:594:U:H2'	22:BA:595:C:C6	2.55	0.42
22:BA:2030:6MZ:H2	22:BA:2499:C:H5"	2.01	0.42
22:BA:2086:U:H2'	22:BA:2087:G:C8	2.54	0.42
22:BA:2467:C:H2'	22:BA:2468:A:O4'	2.18	0.42
22:BA:2698:U:H2'	22:BA:2699:C:C6	2.54	0.42
25:BD:25:THR:OG1	25:BD:191:GLY:O	2.34	0.42
27:BF:147:ASP:OD1	27:BF:150:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:84:ALA:HB1	29:BH:89:LYS:O	2.19	0.42
43:BV:35:GLU:N	43:BV:35:GLU:OE1	2.52	0.42
55:B8:25:C:H2'	55:B8:26:A:O4'	2.19	0.42
1:AA:68:G:O6	1:AA:100:G:O6	2.36	0.42
1:AA:1026:G:C6	1:AA:1027:C:N4	2.87	0.42
1:AA:1106:G:O2'	3:AC:169:ARG:NH2	2.53	0.42
1:AA:1366:C:H2'	1:AA:1367:C:C6	2.55	0.42
6:AF:42:TRP:CZ2	6:AF:102:MET:HG3	2.54	0.42
13:AM:3:ARG:HG2	13:AM:9:ILE:HG12	2.02	0.42
18:AR:38:LYS:HA	18:AR:38:LYS:HD3	1.79	0.42
22:BA:231:A:H2'	22:BA:232:G:O4'	2.20	0.42
22:BA:1007:C:OP1	31:BJ:37:ARG:NH2	2.52	0.42
22:BA:2277:G:H2'	22:BA:2278:A:H5"	2.02	0.42
28:BG:99:LYS:O	28:BG:99:LYS:HG3	2.20	0.42
45:BX:26:LYS:HA	45:BX:26:LYS:HD2	1.97	0.42
56:B9:16:GLU:O	56:B9:20:VAL:HG13	2.19	0.42
56:B9:33:ARG:CD	56:B9:63:LEU:HD11	2.50	0.42
56:B9:86:LEU:O	56:B9:90:ALA:HB3	2.20	0.42
1:AA:463:U:H2'	1:AA:464:U:N1	2.35	0.42
1:AA:744:C:H2'	1:AA:745:G:C8	2.55	0.42
1:AA:748:G:H2'	1:AA:749:A:C8	2.55	0.42
9:AI:57:MET:HA	9:AI:60:LYS:HE2	2.01	0.42
22:BA:84:A:H4'	22:BA:85:G:O5'	2.19	0.42
22:BA:207:A:H2'	22:BA:208:C:O4'	2.20	0.42
22:BA:881:G:N2	22:BA:896:A:H62	2.17	0.42
22:BA:966:G:H2'	22:BA:967:U:C6	2.55	0.42
22:BA:1081:U:H2'	22:BA:1082:U:C6	2.54	0.42
22:BA:2020:A:H5'	48:B0:9:THR:HG21	2.01	0.42
22:BA:2100:G:O6	22:BA:2189:U:C2	2.72	0.42
22:BA:2188:U:H2'	22:BA:2189:U:C5	2.55	0.42
38:BQ:48:ARG:HH11	38:BQ:49:ASP:CG	2.22	0.42
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.35	0.42
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.20	0.42
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.55	0.42
4:AD:28:ILE:HG12	4:AD:34:ILE:HD11	2.02	0.42
4:AD:91:LEU:HD23	4:AD:91:LEU:HA	1.82	0.42
7:AG:129:GLU:HB3	7:AG:131:LYS:NZ	2.35	0.42
11:AK:53:ARG:HD2	11:AK:53:ARG:HA	1.75	0.42
11:AK:126:LYS:HE2	21:AU:37:PHE:HB2	2.00	0.42
12:AL:24:LEU:O	12:AL:27:CYS:HB3	2.20	0.42
22:BA:1410:G:H2'	22:BA:1411:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1790:C:H2'	22:BA:1791:A:C5	2.54	0.42
22:BA:2130:U:H5"	22:BA:2133:G:P	2.60	0.42
29:BH:100:ALA:O	29:BH:104:THR:HG23	2.20	0.42
43:BV:77:VAL:HG22	43:BV:89:ILE:HD12	2.01	0.42
47:BZ:4:THR:HA	47:BZ:39:GLU:HA	2.01	0.42
1:AA:67:C:N4	1:AA:69:G:N1	2.68	0.42
2:AB:59:LYS:O	2:AB:63:ARG:NH1	2.53	0.42
7:AG:42:ILE:HG21	7:AG:116:MET:HG3	2.02	0.42
9:AI:91:ASP:OD2	9:AI:94:LEU:HB2	2.20	0.42
22:BA:1470:A:H2'	22:BA:1471:G:O4'	2.20	0.42
22:BA:1762:A:O5'	22:BA:1762:A:H8	2.03	0.42
22:BA:2474:U:O2'	22:BA:2475:C:OP1	2.34	0.42
22:BA:2796:U:O2'	22:BA:2797:U:H2'	2.19	0.42
23:BB:49:C:H2'	23:BB:50:A:H8	1.85	0.42
25:BD:106:LYS:NZ	25:BD:176:ASP:OD1	2.52	0.42
27:BF:6:ASP:OD1	27:BF:7:TYR:N	2.49	0.42
27:BF:123:ASP:OD2	27:BF:127:ASN:HB2	2.19	0.42
1:AA:523:A:C2	12:AL:88:LYS:HB3	2.55	0.42
1:AA:1003:G:N2	1:AA:1005:A:O5'	2.52	0.42
6:AF:5:GLU:OE1	18:AR:23:TYR:OH	2.24	0.42
10:AJ:8:ILE:HA	10:AJ:99:GLN:O	2.20	0.42
12:AL:100:GLY:N	12:AL:104:CYS:O	2.38	0.42
22:BA:1378:A:O2'	22:BA:1380:G:N7	2.53	0.42
22:BA:2181:U:H2'	22:BA:2182:U:H6	1.85	0.42
22:BA:2395:C:H2'	22:BA:2396:G:O4'	2.19	0.42
22:BA:2529:G:H5'	28:BG:175:LYS:HB3	2.01	0.42
29:BH:57:LYS:O	29:BH:60:GLU:HG3	2.20	0.42
1:AA:324:G:N1	1:AA:327:A:OP2	2.52	0.41
1:AA:460:A:C6	1:AA:461:A:N6	2.88	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.54	0.41
1:AA:864:A:H2'	1:AA:865:A:C8	2.55	0.41
1:AA:999:C:N3	1:AA:1042:A:N6	2.68	0.41
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.85	0.41
1:AA:1355:G:H2'	1:AA:1356:G:C8	2.55	0.41
8:AH:43:GLU:HG3	8:AH:101:ILE:HD13	2.02	0.41
12:AL:107:VAL:CG2	12:AL:110:ARG:HB2	2.49	0.41
13:AM:45:ILE:HD13	13:AM:45:ILE:HA	1.88	0.41
22:BA:138:U:H2'	22:BA:140:C:C5	2.55	0.41
22:BA:279:A:H2'	22:BA:280:U:O4'	2.20	0.41
22:BA:927:A:H2'	22:BA:928:A:C8	2.54	0.41
22:BA:1174:U:H1'	22:BA:1177:G:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1738:G:HO2'	22:BA:1739:A:H8	1.67	0.41
22:BA:2012:G:OP1	40:BS:11:ARG:NH2	2.39	0.41
26:BE:122:GLU:N	26:BE:122:GLU:OE1	2.52	0.41
27:BF:163:ASP:N	27:BF:163:ASP:OD1	2.51	0.41
42:BU:89:ASP:C	42:BU:91:LYS:H	2.24	0.41
56:B9:21:LEU:HD11	56:B9:70:LEU:HD11	2.00	0.41
1:AA:66:A:N6	1:AA:67:C:N4	2.68	0.41
1:AA:100:G:O4'	1:AA:101:A:N9	2.53	0.41
1:AA:458:U:H2'	1:AA:459:A:H8	1.83	0.41
10:AJ:11:LYS:HB2	10:AJ:97:ASP:OD1	2.20	0.41
11:AK:16:VAL:HG12	11:AK:18:ASP:H	1.85	0.41
12:AL:36:ARG:HG2	12:AL:38:TYR:HD1	1.85	0.41
22:BA:361:G:H4'	22:BA:362:A:OP1	2.19	0.41
22:BA:780:G:C2	22:BA:785:G:O6	2.73	0.41
22:BA:1067:A:N6	56:B9:54:GLN:OE1	2.52	0.41
22:BA:1239:G:H2'	22:BA:1240:U:O4'	2.20	0.41
24:BC:157:SER:O	24:BC:160:THR:OG1	2.36	0.41
26:BE:141:MET:HB2	26:BE:143:LEU:HG	2.02	0.41
35:BN:8:ARG:HB3	35:BN:10:LEU:HG	2.01	0.41
1:AA:100:G:N1	1:AA:102:G:C4	2.88	0.41
7:AG:15:ASP:OD1	7:AG:16:PRO:HD2	2.20	0.41
9:AI:49:ARG:O	9:AI:53:GLU:HG2	2.21	0.41
10:AJ:91:ASP:OD1	10:AJ:91:ASP:N	2.49	0.41
11:AK:113:VAL:O	11:AK:113:VAL:HG12	2.20	0.41
22:BA:276:U:O2'	22:BA:277:G:O5'	2.32	0.41
22:BA:1052:C:H2'	22:BA:1053:C:C6	2.55	0.41
22:BA:1141:U:H4'	22:BA:1142:A:O4'	2.20	0.41
1:AA:426:U:H2'	1:AA:427:U:C6	2.55	0.41
1:AA:736:C:OP1	18:AR:61:ARG:NH2	2.49	0.41
2:AB:91:PHE:O	2:AB:150:GLY:HA3	2.21	0.41
16:AP:49:GLY:O	16:AP:50:THR:OG1	2.34	0.41
19:AS:34:TRP:CD1	19:AS:52:HIS:ND1	2.88	0.41
22:BA:1664:A:C2	32:BK:1:MET:HE1	2.55	0.41
22:BA:2070:A:H2'	22:BA:2071:A:O4'	2.20	0.41
22:BA:2743:U:O2'	28:BG:153:ARG:NH1	2.52	0.41
22:BA:2804:U:H2'	22:BA:2805:C:C6	2.55	0.41
23:BB:45:A:C4	23:BB:46:A:C8	3.09	0.41
26:BE:21:ARG:HH11	26:BE:106:LYS:CD	2.33	0.41
26:BE:145:ASP:HB3	26:BE:166:LYS:HB3	2.01	0.41
27:BF:110:ARG:NH2	27:BF:139:PRO:HB3	2.34	0.41
28:BG:4:VAL:O	28:BG:69:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B5:10:SER:HB3	53:B5:15:ILE:CD1	2.50	0.41
56:B9:33:ARG:NE	56:B9:59:GLU:OE1	2.53	0.41
1:AA:2:A:H1'	1:AA:613:C:O2'	2.20	0.41
1:AA:151:A:H5"	1:AA:152:A:OP2	2.20	0.41
1:AA:381:C:H2'	1:AA:382:A:O4'	2.21	0.41
1:AA:441:A:H1'	1:AA:497:G:N2	2.36	0.41
1:AA:559:A:H4'	1:AA:560:A:H3'	2.03	0.41
1:AA:748:G:H2'	1:AA:749:A:H8	1.86	0.41
2:AB:153:ASP:N	2:AB:153:ASP:OD1	2.52	0.41
7:AG:52:GLN:NE2	7:AG:53:ARG:HG3	2.35	0.41
22:BA:1279:G:C6	22:BA:1292:G:C6	3.08	0.41
22:BA:1300:G:H4'	22:BA:1301:A:H5"	2.03	0.41
22:BA:1642:G:H2'	22:BA:1643:G:O4'	2.21	0.41
22:BA:2102:G:N1	22:BA:2188:U:N3	2.62	0.41
27:BF:6:ASP:OD1	27:BF:6:ASP:N	2.53	0.41
28:BG:37:LEU:HD23	28:BG:37:LEU:HA	1.88	0.41
36:BO:76:LYS:O	36:BO:80:GLU:OE1	2.39	0.41
38:BQ:76:TYR:CZ	38:BQ:80:ILE:HG13	2.55	0.41
39:BR:78:ARG:HE	39:BR:78:ARG:HB2	1.69	0.41
40:BS:7:HIS:ND1	40:BS:10:ALA:HB2	2.36	0.41
56:B9:349:LEU:HD23	56:B9:349:LEU:HA	1.84	0.41
1:AA:208:U:H3'	1:AA:210:C:N4	2.34	0.41
1:AA:383:A:O5'	1:AA:383:A:H8	2.04	0.41
1:AA:411:A:P	4:AD:26:ARG:HH12	2.43	0.41
1:AA:552:U:H2'	1:AA:553:A:H8	1.86	0.41
1:AA:954:G:H2'	1:AA:955:U:O4'	2.21	0.41
3:AC:6:HIS:CE1	3:AC:8:ASN:HB3	2.56	0.41
3:AC:33:LEU:HD23	3:AC:33:LEU:HA	1.92	0.41
5:AE:15:LEU:HD12	5:AE:37:THR:HG22	2.03	0.41
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.20	0.41
22:BA:1528:A:H2'	22:BA:1529:G:O4'	2.20	0.41
22:BA:2137:U:C2	22:BA:2138:G:N7	2.88	0.41
22:BA:2189:U:C2'	22:BA:2190:G:H8	2.25	0.41
29:BH:72:ILE:HG13	29:BH:73:ASN:N	2.35	0.41
30:BI:58:ASP:OD2	30:BI:58:ASP:N	2.53	0.41
33:BL:109:LYS:HG2	33:BL:126:ARG:HB2	2.02	0.41
34:BM:24:THR:HG22	34:BM:99:GLY:O	2.20	0.41
1:AA:477:C:H2'	1:AA:479:U:O4'	2.20	0.41
1:AA:494:G:O2'	1:AA:496:A:H1'	2.20	0.41
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.49	0.41
1:AA:1320:C:N3	19:AS:36:ARG:NH1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:79:LYS:O	3:AC:80:LYS:HG3	2.20	0.41
3:AC:191:THR:HG22	3:AC:193:TYR:H	1.84	0.41
6:AF:3:HIS:ND1	6:AF:65:GLU:CD	2.74	0.41
14:AN:73:PHE:CZ	14:AN:78:GLY:HA2	2.56	0.41
19:AS:29:LYS:HD2	19:AS:30:PRO:O	2.21	0.41
22:BA:545:U:O2'	22:BA:546:U:O5'	2.26	0.41
22:BA:729:G:C6	24:BC:207:LYS:HB2	2.56	0.41
22:BA:1185:G:H5"	22:BA:1186:G:OP1	2.21	0.41
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.56	0.41
22:BA:2148:G:C2	22:BA:2149:U:C4	3.09	0.41
23:BB:94:A:H2'	23:BB:95:U:O4'	2.20	0.41
53:B5:10:SER:HA	53:B5:11:LYS:HB2	2.02	0.41
1:AA:455:G:H2'	1:AA:456:A:C8	2.56	0.41
1:AA:594:U:H2'	1:AA:595:A:O4'	2.20	0.41
1:AA:1118:U:O3'	9:AI:85:ARG:NH2	2.43	0.41
1:AA:1141:C:H2'	1:AA:1142:G:C8	2.55	0.41
1:AA:1261:A:C5	1:AA:1262:C:C5	3.09	0.41
1:AA:1263:C:H2'	1:AA:1264:U:C6	2.56	0.41
4:AD:103:TYR:CE1	4:AD:110:THR:HA	2.55	0.41
4:AD:144:SER:HB3	4:AD:179:GLU:HB2	2.02	0.41
7:AG:25:LYS:O	7:AG:29:ILE:HG12	2.20	0.41
7:AG:31:MET:HE1	7:AG:34:GLY:HA2	2.03	0.41
22:BA:718:A:H2'	22:BA:719:C:O4'	2.20	0.41
22:BA:2392:A:C2	33:BL:55:MET:SD	3.13	0.41
26:BE:46:GLN:HB2	26:BE:86:ALA:HB1	2.02	0.41
56:B9:85:GLU:HG3	56:B9:89:GLU:CD	2.41	0.41
1:AA:88:U:H1'	1:AA:89:U:H5	1.85	0.41
1:AA:185:U:H2'	1:AA:186:C:H6	1.84	0.41
1:AA:323:U:H2'	1:AA:324:G:O4'	2.21	0.41
1:AA:858:G:O6	1:AA:869:G:H3'	2.21	0.41
1:AA:1338:G:O2'	55:B8:41:A:H4'	2.21	0.41
3:AC:50:ALA:O	3:AC:70:THR:OG1	2.39	0.41
4:AD:198:HIS:HA	4:AD:201:VAL:HG22	2.02	0.41
13:AM:57:ARG:NH1	30:BI:35:ASP:OD2	2.54	0.41
20:AT:9:LYS:O	20:AT:13:GLN:HG3	2.21	0.41
22:BA:2178:C:H2'	22:BA:2179:C:C6	2.56	0.41
22:BA:2489:U:H2'	22:BA:2490:G:O4'	2.20	0.41
23:BB:24:G:H8	23:BB:24:G:H2'	1.78	0.41
23:BB:51:G:O2'	23:BB:52:A:H5'	2.21	0.41
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	2.03	0.41
40:BS:2:GLU:HG2	40:BS:106:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:27:TYR:CD1	56:B9:70:LEU:HD12	2.56	0.41
1:AA:76:G:C5	1:AA:77:A:N7	2.89	0.41
1:AA:1006:G:H2'	1:AA:1007:U:O4'	2.21	0.41
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.55	0.41
12:AL:4:VAL:CG2	17:AQ:34:TYR:HB3	2.50	0.41
12:AL:108:LYS:HA	12:AL:108:LYS:HD2	1.89	0.41
21:AU:25:LYS:HE2	21:AU:25:LYS:HA	2.03	0.41
22:BA:2137:U:H2'	22:BA:2138:G:C8	2.56	0.41
22:BA:2662:A:O5'	22:BA:2662:A:H8	2.04	0.41
27:BF:11:GLU:HG2	27:BF:12:VAL:N	2.35	0.41
28:BG:54:PRO:HG3	28:BG:62:TRP:CE2	2.56	0.41
29:BH:114:GLU:N	29:BH:114:GLU:OE2	2.54	0.41
56:B9:302:LYS:NZ	56:B9:303:LYS:HD3	2.36	0.41
1:AA:222:C:H2'	1:AA:223:A:H8	1.86	0.40
2:AB:115:LYS:HE2	2:AB:115:LYS:HB3	1.77	0.40
9:AI:96:SER:O	9:AI:100:LYS:HG2	2.20	0.40
13:AM:83:LEU:CD2	19:AS:74:PHE:HE1	2.34	0.40
22:BA:727:A:O2'	22:BA:728:G:H5'	2.22	0.40
22:BA:1230:A:H2'	22:BA:1231:U:O4'	2.22	0.40
22:BA:1394:U:H4'	22:BA:1603:A:H4'	2.04	0.40
23:BB:45:A:C8	27:BF:92:ARG:NH2	2.89	0.40
26:BE:175:ILE:O	26:BE:175:ILE:HG13	2.20	0.40
31:BJ:49:ASP:OD2	31:BJ:121:LYS:NZ	2.53	0.40
36:BO:26:LEU:HD23	36:BO:92:PHE:HD1	1.87	0.40
36:BO:56:LYS:HA	36:BO:56:LYS:HD3	1.77	0.40
38:BQ:3:ARG:HH21	38:BQ:3:ARG:HD3	1.72	0.40
43:BV:2:PHE:HB2	43:BV:61:LEU:HD22	2.03	0.40
56:B9:51:GLU:HG2	56:B9:52:ARG:N	2.36	0.40
56:B9:121:GLY:C	56:B9:123:TYR:H	2.25	0.40
1:AA:377:G:H2'	1:AA:378:G:H8	1.86	0.40
1:AA:511:C:C2	1:AA:512:U:C5	3.09	0.40
1:AA:652:U:O4	1:AA:752:G:O2'	2.30	0.40
1:AA:900:A:H2'	1:AA:901:A:C8	2.57	0.40
1:AA:946:A:H2'	1:AA:947:G:H8	1.86	0.40
1:AA:1122:U:H2'	1:AA:1123:U:C6	2.55	0.40
1:AA:1373:G:N7	9:AI:13:LYS:NZ	2.65	0.40
13:AM:4:ILE:HG22	13:AM:5:ALA:N	2.32	0.40
22:BA:721:A:H2'	22:BA:722:A:C8	2.56	0.40
22:BA:1073:A:O5'	22:BA:1073:A:C8	2.73	0.40
22:BA:1438:U:H2'	22:BA:1439:A:H8	1.86	0.40
22:BA:2137:U:H2'	22:BA:2138:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2148:G:H2'	22:BA:2149:U:C6	2.56	0.40
26:BE:21:ARG:O	26:BE:114:ARG:NH2	2.53	0.40
56:B9:64:GLU:O	56:B9:68:ASP:HB2	2.21	0.40
1:AA:69:G:N2	1:AA:102:G:C6	2.89	0.40
1:AA:102:G:C5	1:AA:103:U:C4	3.09	0.40
1:AA:373:A:H2'	1:AA:374:A:H8	1.85	0.40
1:AA:459:A:H2'	1:AA:460:A:H8	1.83	0.40
1:AA:737:C:H2'	1:AA:738:C:H6	1.86	0.40
13:AM:62:LYS:HE2	13:AM:62:LYS:HA	2.03	0.40
19:AS:17:LYS:HD3	19:AS:17:LYS:HA	1.91	0.40
22:BA:276:U:O2'	22:BA:277:G:O4'	2.38	0.40
22:BA:1263:U:OP1	48:B0:13:ARG:NH1	2.55	0.40
35:BN:58:ASP:OD1	35:BN:63:ARG:NH1	2.42	0.40
1:AA:66:A:N6	1:AA:104:G:C2	2.90	0.40
1:AA:457:G:N2	1:AA:474:G:H1	2.19	0.40
1:AA:457:G:H1	1:AA:474:G:H1	1.69	0.40
1:AA:685:G:O2'	1:AA:686:U:H5'	2.21	0.40
4:AD:78:GLU:OE2	4:AD:81:ARG:NE	2.45	0.40
7:AG:131:LYS:HE2	7:AG:131:LYS:HB2	1.97	0.40
13:AM:66:GLU:CG	13:AM:67:GLY:H	2.30	0.40
17:AQ:68:SER:OG	17:AQ:69:LYS:N	2.54	0.40
22:BA:1183:U:H2'	22:BA:1184:U:C6	2.57	0.40
22:BA:2101:A:C2	22:BA:2102:G:C5	3.08	0.40
22:BA:2136:G:C6	22:BA:2156:G:C2	3.10	0.40
24:BC:75:PRO:HG2	24:BC:97:LYS:CG	2.51	0.40
30:BI:42:PRO:O	30:BI:46:GLY:HA3	2.21	0.40
33:BL:131:ALA:O	33:BL:135:ILE:HG13	2.21	0.40
41:BT:69:ARG:HH11	41:BT:69:ARG:HD3	1.77	0.40
43:BV:89:ILE:HD12	43:BV:89:ILE:HG23	1.84	0.40
1:AA:195:A:OP1	20:AT:60:ARG:NH1	2.55	0.40
1:AA:459:A:N6	1:AA:460:A:N6	2.70	0.40
1:AA:1198:G:H2'	1:AA:1199:U:C6	2.57	0.40
7:AG:148:ASN:ND2	11:AK:56:ARG:HH21	2.19	0.40
14:AN:16:ALA:HA	14:AN:55:SER:HA	2.03	0.40
21:AU:21:ARG:HD2	21:AU:24:GLU:OE2	2.22	0.40
22:BA:1079:C:C2	22:BA:1080:A:C8	3.10	0.40
22:BA:1392:A:H62	41:BT:18:GLU:HG3	1.86	0.40
22:BA:2175:C:H2'	22:BA:2176:A:C8	2.57	0.40
22:BA:2737:G:H2'	22:BA:2738:A:C8	2.57	0.40
35:BN:106:ASP:N	35:BN:106:ASP:OD1	2.54	0.40
54:B7:2:G:N3	54:B7:2:G:H2'	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:B9:244:TYR:HE1	56:B9:262:ARG:HB2	1.87	0.40
56:B9:299:GLU:O	56:B9:303:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	AD	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	AE	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	AF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	AG	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	7	13
11	AK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	AL	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
13	AM	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
14	AN	99/102 (97%)	84 (85%)	15 (15%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	52
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
35	BN	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	BO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	BP	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	15	32
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
49	B1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	6
52	B4	36/38 (95%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	B5	15/17 (88%)	13 (87%)	2 (13%)	0	100 100
56	B9	344/365 (94%)	325 (94%)	19 (6%)	0	100 100
All	All	5934/6296 (94%)	5626 (95%)	302 (5%)	6 (0%)	54 75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN
42	BU	8	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	186/199 (94%)	186 (100%)	0	100 100
3	AC	170/190 (90%)	168 (99%)	2 (1%)	71 87
4	AD	172/173 (99%)	171 (99%)	1 (1%)	86 95
5	AE	118/126 (94%)	118 (100%)	0	100 100
6	AF	92/116 (79%)	92 (100%)	0	100 100
7	AG	124/147 (84%)	124 (100%)	0	100 100
8	AH	104/105 (99%)	104 (100%)	0	100 100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	76 90
10	AJ	87/90 (97%)	87 (100%)	0	100 100
11	AK	90/99 (91%)	89 (99%)	1 (1%)	73 88
12	AL	102/103 (99%)	102 (100%)	0	100 100
13	AM	92/96 (96%)	92 (100%)	0	100 100
14	AN	79/84 (94%)	78 (99%)	1 (1%)	69 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	AO	76/77 (99%)	75 (99%)	1 (1%)	69 86
16	AP	65/65 (100%)	65 (100%)	0	100 100
17	AQ	74/78 (95%)	74 (100%)	0	100 100
18	AR	48/65 (74%)	47 (98%)	1 (2%)	53 77
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67 85
20	AT	65/66 (98%)	65 (100%)	0	100 100
21	AU	48/61 (79%)	48 (100%)	0	100 100
24	BC	216/218 (99%)	216 (100%)	0	100 100
25	BD	163/163 (100%)	161 (99%)	2 (1%)	71 87
26	BE	165/165 (100%)	165 (100%)	0	100 100
27	BF	148/150 (99%)	148 (100%)	0	100 100
28	BG	137/138 (99%)	137 (100%)	0	100 100
29	BH	114/114 (100%)	114 (100%)	0	100 100
30	BI	59/62 (95%)	59 (100%)	0	100 100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78 91
32	BK	104/104 (100%)	104 (100%)	0	100 100
33	BL	103/103 (100%)	103 (100%)	0	100 100
34	BM	108/108 (100%)	108 (100%)	0	100 100
35	BN	98/103 (95%)	98 (100%)	0	100 100
36	BO	87/87 (100%)	86 (99%)	1 (1%)	73 88
37	BP	99/100 (99%)	98 (99%)	1 (1%)	76 90
38	BQ	89/90 (99%)	89 (100%)	0	100 100
39	BR	84/84 (100%)	84 (100%)	0	100 100
40	BS	93/93 (100%)	93 (100%)	0	100 100
41	BT	80/84 (95%)	80 (100%)	0	100 100
42	BU	83/85 (98%)	83 (100%)	0	100 100
43	BV	78/78 (100%)	78 (100%)	0	100 100
44	BW	57/63 (90%)	57 (100%)	0	100 100
45	BX	67/68 (98%)	67 (100%)	0	100 100
46	BY	54/55 (98%)	54 (100%)	0	100 100
47	BZ	48/49 (98%)	48 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	B0	47/48 (98%)	47 (100%)	0	100 100
49	B1	45/49 (92%)	45 (100%)	0	100 100
50	B2	38/38 (100%)	37 (97%)	1 (3%)	46 72
51	B3	51/52 (98%)	51 (100%)	0	100 100
52	B4	34/34 (100%)	34 (100%)	0	100 100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19 39
56	B9	298/311 (96%)	296 (99%)	2 (1%)	84 94
All	All	4948/5155 (96%)	4930 (100%)	18 (0%)	91 97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	79	LYS
3	AC	80	LYS
4	AD	128	ARG
9	AI	106	ARG
11	AK	13	ARG
14	AN	22	LYS
15	AO	80	GLN
18	AR	73	ARG
19	AS	81	ARG
25	BD	33	ARG
25	BD	128	ARG
31	BJ	128	ASN
36	BO	63	LYS
37	BP	37	LYS
50	B2	41	ARG
53	B5	24	PRO
56	B9	33	ARG
56	B9	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	122	GLN
4	AD	152	GLN
7	AG	148	ASN
8	AH	118	GLN

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Mol	Chain	Res	Type
11	AK	119	ASN
26	BE	97	ASN
41	BT	48	GLN
56	B9	281	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	241 (15%)	8 (0%)
22	BA	2890/2897 (99%)	438 (15%)	24 (0%)
23	BB	119/120 (99%)	15 (12%)	1 (0%)
54	B7	8/10 (80%)	2 (25%)	0
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4623/4638 (99%)	708 (15%)	35 (0%)

All (708) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	19	A
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	44	A
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	58	C
1	AA	59	A
1	AA	68	G
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	76	G
1	AA	78	A
1	AA	81	A
1	AA	82	G
1	AA	83	C

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Mol	Chain	Res	Type
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	90	C
1	AA	92	U
1	AA	99	C
1	AA	100	G
1	AA	101	A
1	AA	102	G
1	AA	116	A
1	AA	119	A
1	AA	120	A
1	AA	121	U
1	AA	122	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	151	A
1	AA	161	A
1	AA	163	C
1	AA	164	G
1	AA	181	A
1	AA	182	A
1	AA	189	A
1	AA	197	A
1	AA	204	G
1	AA	210	C
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	299	G
1	AA	306	A
1	AA	321	A
1	AA	327	A
1	AA	328	C
1	AA	344	A
1	AA	352	C

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Mol	Chain	Res	Type
1	AA	353	A
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	429	U
1	AA	437	U
1	AA	439	U
1	AA	463	U
1	AA	465	A
1	AA	468	A
1	AA	474	G
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	482	A
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	499	A
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	518	C
1	AA	521	G
1	AA	527	G7M
1	AA	529	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	560	A
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G

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Mol	Chain	Res	Type
1	AA	579	A
1	AA	588	G
1	AA	596	A
1	AA	600	A
1	AA	633	G
1	AA	653	U
1	AA	665	A
1	AA	702	A
1	AA	703	G
1	AA	718	A
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	724	G
1	AA	734	G
1	AA	755	G
1	AA	758	C
1	AA	760	G
1	AA	777	A
1	AA	790	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	864	A
1	AA	889	A
1	AA	900	A
1	AA	902	G
1	AA	914	A
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	958	A
1	AA	960	U

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Mol	Chain	Res	Type
1	AA	966	2MG
1	AA	969	A
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1022	A
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1042	A
1	AA	1045	C
1	AA	1046	A
1	AA	1065	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1132	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1146	A
1	AA	1151	A
1	AA	1154	G
1	AA	1157	A
1	AA	1159	U
1	AA	1169	A
1	AA	1173	U
1	AA	1184	G
1	AA	1191	A

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Mol	Chain	Res	Type
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1212	U
1	AA	1213	A
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1248	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1285	A
1	AA	1287	A
1	AA	1288	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1335	U
1	AA	1336	C
1	AA	1340	A
1	AA	1346	A
1	AA	1363	A
1	AA	1370	G
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1432	G
1	AA	1441	A
1	AA	1446	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G

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Mol	Chain	Res	Type
1	AA	1499	A
1	AA	1502	A
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
22	BA	10	A
22	BA	12	U
22	BA	15	G
22	BA	51	G
22	BA	61	C
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	101	A
22	BA	103	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	125	A
22	BA	143	C
22	BA	163	C
22	BA	165	A
22	BA	167	A
22	BA	181	A
22	BA	193	U
22	BA	196	A
22	BA	197	A
22	BA	199	A
22	BA	204	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	224	U
22	BA	233	A
22	BA	241	A
22	BA	248	G
22	BA	264	C

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Mol	Chain	Res	Type
22	BA	265	A
22	BA	272	A
22	BA	274	C
22	BA	275	C
22	BA	276	U
22	BA	277	G
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	322	A
22	BA	330	A
22	BA	345	A
22	BA	360	U
22	BA	361	G
22	BA	385	C
22	BA	386	G
22	BA	396	G
22	BA	404	A
22	BA	406	G
22	BA	407	G
22	BA	411	G
22	BA	412	A
22	BA	417	C
22	BA	425	G
22	BA	428	A
22	BA	435	C
22	BA	480	A
22	BA	481	G
22	BA	489	G
22	BA	491	G
22	BA	503	A
22	BA	505	A
22	BA	509	C
22	BA	510	C
22	BA	530	G
22	BA	532	A
22	BA	546	U
22	BA	547	A
22	BA	549	G
22	BA	550	C
22	BA	557	C
22	BA	563	A

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Mol	Chain	Res	Type
22	BA	568	U
22	BA	573	U
22	BA	575	A
22	BA	588	U
22	BA	592	A
22	BA	603	A
22	BA	614	A
22	BA	615	U
22	BA	616	A
22	BA	637	A
22	BA	644	A
22	BA	645	C
22	BA	646	U
22	BA	647	G
22	BA	653	U
22	BA	654	A
22	BA	655	A
22	BA	668	A
22	BA	685	A
22	BA	686	U
22	BA	688	U
22	BA	696	G
22	BA	711	G
22	BA	717	C
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
22	BA	762	U
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	789	A
22	BA	790	U
22	BA	791	C
22	BA	792	A
22	BA	802	A
22	BA	805	G
22	BA	806	C

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Mol	Chain	Res	Type
22	BA	812	C
22	BA	827	U
22	BA	828	U
22	BA	846	U
22	BA	847	U
22	BA	859	G
22	BA	866	A
22	BA	883	G
22	BA	884	U
22	BA	885	C
22	BA	896	A
22	BA	905	A
22	BA	910	A
22	BA	914	G
22	BA	945	A
22	BA	946	C
22	BA	961	C
22	BA	973	A
22	BA	974	G
22	BA	983	A
22	BA	985	C
22	BA	996	A
22	BA	1005	C
22	BA	1012	U
22	BA	1013	C
22	BA	1025	G
22	BA	1026	G
22	BA	1033	U
22	BA	1046	A
22	BA	1047	G
22	BA	1054	A
22	BA	1057	A
22	BA	1061	U
22	BA	1067	A
22	BA	1069	A
22	BA	1070	A
22	BA	1071	G
22	BA	1073	A
22	BA	1075	C
22	BA	1076	C
22	BA	1077	A
22	BA	1083	U

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Mol	Chain	Res	Type
22	BA	1084	A
22	BA	1085	A
22	BA	1088	A
22	BA	1097	U
22	BA	1101	U
22	BA	1110	G
22	BA	1111	A
22	BA	1112	G
22	BA	1126	A
22	BA	1128	G
22	BA	1130	U
22	BA	1132	U
22	BA	1133	A
22	BA	1134	A
22	BA	1135	C
22	BA	1142	A
22	BA	1156	A
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1187	G
22	BA	1189	A
22	BA	1204	A
22	BA	1205	A
22	BA	1206	G
22	BA	1212	G
22	BA	1247	A
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1273	U
22	BA	1274	A
22	BA	1275	A
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A
22	BA	1313	U
22	BA	1321	A

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Mol	Chain	Res	Type
22	BA	1329	U
22	BA	1352	U
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1392	A
22	BA	1393	A
22	BA	1395	A
22	BA	1416	G
22	BA	1428	C
22	BA	1429	G
22	BA	1452	G
22	BA	1453	A
22	BA	1458	U
22	BA	1460	U
22	BA	1478	G
22	BA	1482	G
22	BA	1494	A
22	BA	1508	A
22	BA	1515	A
22	BA	1524	G
22	BA	1535	A
22	BA	1537	G
22	BA	1554	U
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1606	C
22	BA	1608	A
22	BA	1609	A
22	BA	1610	A
22	BA	1630	A
22	BA	1634	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1664	A
22	BA	1674	G
22	BA	1675	C
22	BA	1677	A
22	BA	1729	U
22	BA	1730	C

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Mol	Chain	Res	Type
22	BA	1732	C
22	BA	1733	G
22	BA	1744	A
22	BA	1754	A
22	BA	1757	A
22	BA	1758	U
22	BA	1759	A
22	BA	1764	C
22	BA	1773	A
22	BA	1782	U
22	BA	1786	A
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1809	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1848	A
22	BA	1862	G
22	BA	1870	C
22	BA	1871	A
22	BA	1872	A
22	BA	1900	A
22	BA	1905	C
22	BA	1906	G
22	BA	1913	A
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1936	A
22	BA	1937	A
22	BA	1938	A
22	BA	1955	U
22	BA	1960	A
22	BA	1966	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1991	U

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Mol	Chain	Res	Type
22	BA	1993	U
22	BA	1996	C
22	BA	2006	C
22	BA	2023	C
22	BA	2031	A
22	BA	2032	G
22	BA	2033	A
22	BA	2036	C
22	BA	2043	C
22	BA	2052	A
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2077	A
22	BA	2080	A
22	BA	2093	G
22	BA	2097	A
22	BA	2101	A
22	BA	2110	G
22	BA	2111	U
22	BA	2112	G
22	BA	2113	U
22	BA	2114	A
22	BA	2115	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2121	G
22	BA	2125	G
22	BA	2126	A
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2136	G
22	BA	2137	U
22	BA	2142	A
22	BA	2145	C
22	BA	2147	A

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Mol	Chain	Res	Type
22	BA	2154	A
22	BA	2157	G
22	BA	2158	A
22	BA	2159	G
22	BA	2161	C
22	BA	2162	G
22	BA	2164	C
22	BA	2168	G
22	BA	2169	A
22	BA	2170	A
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2183	A
22	BA	2184	A
22	BA	2186	G
22	BA	2188	U
22	BA	2189	U
22	BA	2191	A
22	BA	2198	A
22	BA	2203	U
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2259	U
22	BA	2261	C
22	BA	2267	A
22	BA	2269	G
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2298	A
22	BA	2303	G
22	BA	2305	U
22	BA	2308	G
22	BA	2322	A
22	BA	2325	G
22	BA	2327	A
22	BA	2333	A

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Mol	Chain	Res	Type
22	BA	2336	A
22	BA	2340	A
22	BA	2347	C
22	BA	2350	C
22	BA	2383	G
22	BA	2385	C
22	BA	2396	G
22	BA	2402	U
22	BA	2406	A
22	BA	2425	A
22	BA	2429	G
22	BA	2435	A
22	BA	2440	C
22	BA	2441	U
22	BA	2448	A
22	BA	2459	A
22	BA	2469	A
22	BA	2475	C
22	BA	2476	A
22	BA	2491	U
22	BA	2502	G
22	BA	2504	PSU
22	BA	2505	G
22	BA	2507	C
22	BA	2518	A
22	BA	2529	G
22	BA	2534	A
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2572	A
22	BA	2573	C
22	BA	2577	A
22	BA	2582	G
22	BA	2602	A
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2629	U
22	BA	2630	G
22	BA	2654	A
22	BA	2663	G

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Mol	Chain	Res	Type
22	BA	2689	U
22	BA	2690	U
22	BA	2705	A
22	BA	2713	U
22	BA	2714	G
22	BA	2718	G
22	BA	2724	U
22	BA	2726	A
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2751	G
22	BA	2778	A
22	BA	2799	A
22	BA	2820	A
22	BA	2821	A
22	BA	2849	U
22	BA	2850	A
22	BA	2861	U
22	BA	2873	A
22	BA	2874	C
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2891	U
22	BA	2893	A
23	BB	13	G
23	BB	24	G
23	BB	26	C
23	BB	30	C
23	BB	35	C
23	BB	42	C
23	BB	44	G
23	BB	56	G
23	BB	57	A
23	BB	66	A
23	BB	68	C
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	B7	4	C

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Mol	Chain	Res	Type
54	B7	10	U
55	B8	3	G
55	B8	4	U
55	B8	5	G
55	B8	6	A
55	B8	14	A
55	B8	17	C
55	B8	19	G
55	B8	21	A
55	B8	22	G
55	B8	74	C
55	B8	75	C
55	B8	76	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	69	G
1	AA	99	C
1	AA	100	G
1	AA	119	A
1	AA	428	G
1	AA	1225	A
1	AA	1299	A
1	AA	1493	A
22	BA	125	A
22	BA	196	A
22	BA	199	A
22	BA	276	U
22	BA	685	A
22	BA	764	A
22	BA	784	G
22	BA	984	A
22	BA	1067	A
22	BA	1175	A
22	BA	1247	A
22	BA	1253	A
22	BA	1392	A
22	BA	1608	A
22	BA	1847	A
22	BA	1900	A
22	BA	1913	A

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Mol	Chain	Res	Type
22	BA	2158	A
22	BA	2183	A
22	BA	2211	A
22	BA	2474	U
22	BA	2518	A
22	BA	2820	A
22	BA	2873	A
23	BB	66	A
55	B8	2	G
55	B8	3	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

37 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	6MZ	BA	1618	22	18,25,26	2.84	5 (27%)	16,36,39	2.95	4 (25%)
1	5MC	AA	967	1	18,22,23	3.36	7 (38%)	26,32,35	1.12	1 (3%)
22	5MU	BA	747	40,22	19,22,23	0.76	0	28,32,35	1.13	2 (7%)
22	3TD	BA	1915	56,22	18,22,23	4.04	7 (38%)	22,32,35	1.75	3 (13%)
22	PSU	BA	2604	22	18,21,22	3.40	6 (33%)	22,30,33	2.74	6 (27%)
22	G7M	BA	2069	58,22	20,26,27	1.98	5 (25%)	17,39,42	1.22	2 (11%)
22	PSU	BA	1917	22	18,21,22	3.88	6 (33%)	22,30,33	1.96	5 (22%)
22	OMG	BA	2251	55,58,22	18,26,27	2.14	5 (27%)	19,38,41	1.50	5 (26%)
22	2MA	BA	2503	58,22,57	17,25,26	2.15	5 (29%)	17,37,40	1.56	4 (23%)
22	5MU	BA	1939	58,22	19,22,23	1.05	3 (15%)	28,32,35	1.32	4 (14%)
1	4OC	AA	1402	1,57	20,23,24	2.76	8 (40%)	26,32,35	0.96	2 (7%)
22	PSU	BA	2605	22	18,21,22	3.54	8 (44%)	22,30,33	2.06	4 (18%)
1	MA6	AA	1518	1	18,26,27	1.44	5 (27%)	19,38,41	3.33	2 (10%)
22	6MZ	BA	2030	22	18,25,26	2.87	6 (33%)	16,36,39	2.91	4 (25%)
1	PSU	AA	516	1,57	18,21,22	4.01	7 (38%)	22,30,33	1.98	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	PSU	BA	2580	22	18,21,22	3.58	7 (38%)	22,30,33	1.97	4 (18%)
22	OMU	BA	2552	22,57	19,22,23	2.56	7 (36%)	26,31,34	2.05	6 (23%)
22	PSU	BA	2504	58,22	18,21,22	3.52	6 (33%)	22,30,33	1.74	4 (18%)
1	2MG	AA	966	1	18,26,27	2.37	7 (38%)	16,38,41	1.41	4 (25%)
1	2MG	AA	1207	58,1	18,26,27	2.37	7 (38%)	16,38,41	1.43	3 (18%)
1	2MG	AA	1516	1	18,26,27	2.21	6 (33%)	16,38,41	1.81	4 (25%)
12	D2T	AL	89	12	7,9,10	1.02	0	6,11,13	2.65	3 (50%)
22	5MC	BA	1962	58,22	18,22,23	2.90	7 (38%)	26,32,35	1.10	2 (7%)
1	5MC	AA	1407	1	18,22,23	3.14	7 (38%)	26,32,35	1.22	2 (7%)
22	PSU	BA	2457	22	18,21,22	3.44	7 (38%)	22,30,33	2.45	5 (22%)
22	PSU	BA	1911	22	18,21,22	3.98	7 (38%)	22,30,33	2.22	5 (22%)
22	OMC	BA	2498	22,57	19,22,23	2.45	7 (36%)	26,31,34	0.97	2 (7%)
22	1MG	BA	745	22	18,26,27	2.41	5 (27%)	19,39,42	1.52	3 (15%)
22	2MG	BA	1835	22	18,26,27	2.05	5 (27%)	16,38,41	1.78	4 (25%)
34	4D4	BM	81	34	9,11,12	2.44	4 (44%)	8,13,15	1.26	1 (12%)
1	G7M	AA	527	58,1	20,26,27	2.31	6 (30%)	17,39,42	1.26	1 (5%)
22	PSU	BA	955	22	18,21,22	3.56	6 (33%)	22,30,33	2.31	5 (22%)
22	2MG	BA	2445	22	18,26,27	2.12	5 (27%)	16,38,41	2.12	4 (25%)
22	PSU	BA	746	22,57	18,21,22	3.95	8 (44%)	22,30,33	1.73	6 (27%)
25	MEQ	BD	150	25	8,9,10	1.43	2 (25%)	5,10,12	1.50	1 (20%)
1	UR3	AA	1498	1	19,22,23	2.91	8 (42%)	26,32,35	1.43	2 (7%)
1	MA6	AA	1519	1	18,26,27	1.39	3 (16%)	19,38,41	3.70	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MU	BA	747	40,22	-	3/7/25/26	0/2/2/2
22	3TD	BA	1915	56,22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	58,22	-	2/3/25/26	0/3/3/3
22	PSU	BA	1917	22	-	1/7/25/26	0/2/2/2
22	OMG	BA	2251	55,58,22	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	2MA	BA	2503	58,22,57	-	2/3/25/26	0/3/3/3
22	5MU	BA	1939	58,22	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1,57	-	2/9/29/30	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
1	PSU	AA	516	1,57	-	1/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	OMU	BA	2552	22,57	-	0/9/27/28	0/2/2/2
22	PSU	BA	2504	58,22	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	58,1	-	0/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	5MC	BA	1962	58,22	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	22,57	-	0/9/27/28	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	2/11/12/14	-
1	G7M	AA	527	58,1	-	2/3/25/26	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	746	22,57	-	3/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	4/8/9/11	-
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	11.61	1.48	1.35
22	BA	1911	PSU	C6-C5	10.71	1.47	1.35
22	BA	1917	PSU	C6-C5	10.44	1.47	1.35
1	AA	516	PSU	C6-C5	10.41	1.47	1.35
22	BA	2030	6MZ	C6-N6	10.36	1.52	1.35
22	BA	1618	6MZ	C6-N6	10.32	1.51	1.35
22	BA	746	PSU	C6-C5	10.24	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2580	PSU	C6-C5	9.81	1.46	1.35
22	BA	2605	PSU	C6-C5	9.54	1.46	1.35
22	BA	2504	PSU	C6-C5	9.53	1.46	1.35
22	BA	1911	PSU	C2-N1	9.26	1.49	1.36
22	BA	955	PSU	C6-C5	9.18	1.46	1.35
22	BA	2457	PSU	C6-C5	9.15	1.46	1.35
1	AA	516	PSU	C2-N1	9.15	1.49	1.36
22	BA	2604	PSU	C6-C5	8.94	1.45	1.35
22	BA	746	PSU	C2-N1	8.88	1.48	1.36
22	BA	1917	PSU	C2-N1	8.61	1.48	1.36
1	AA	967	5MC	C6-C5	8.44	1.48	1.34
22	BA	1915	3TD	C2-N1	8.41	1.48	1.37
1	AA	1407	5MC	C6-C5	8.40	1.48	1.34
22	BA	955	PSU	C2-N1	7.86	1.47	1.36
1	AA	1498	UR3	C2-N1	7.79	1.49	1.38
22	BA	2580	PSU	C2-N1	7.78	1.47	1.36
22	BA	2504	PSU	C2-N1	7.72	1.47	1.36
22	BA	2457	PSU	C2-N1	7.69	1.47	1.36
22	BA	2604	PSU	C2-N1	7.50	1.46	1.36
22	BA	2605	PSU	C2-N1	7.40	1.46	1.36
22	BA	1962	5MC	C6-C5	7.21	1.46	1.34
1	AA	516	PSU	C2-N3	6.81	1.49	1.37
22	BA	746	PSU	C2-N3	6.45	1.48	1.37
22	BA	1917	PSU	C2-N3	6.39	1.48	1.37
1	AA	967	5MC	C4-N3	6.19	1.44	1.34
22	BA	1911	PSU	C2-N3	6.16	1.48	1.37
22	BA	2605	PSU	C2-N3	6.02	1.47	1.37
22	BA	2604	PSU	C2-N3	5.96	1.47	1.37
22	BA	2503	2MA	C2-N3	5.96	1.43	1.31
1	AA	1402	4OC	C6-C5	5.88	1.48	1.35
22	BA	955	PSU	C2-N3	5.87	1.47	1.37
1	AA	1402	4OC	C4-N3	5.76	1.42	1.32
1	AA	967	5MC	C2-N3	5.75	1.48	1.36
22	BA	745	1MG	C2-N3	5.73	1.44	1.34
22	BA	2504	PSU	C2-N3	5.65	1.47	1.37
22	BA	2457	PSU	C2-N3	5.58	1.47	1.37
22	BA	2552	OMU	C2-N1	5.48	1.47	1.38
22	BA	2552	OMU	C2-N3	5.40	1.47	1.38
34	BM	81	4D4	CZ-NE	5.33	1.43	1.33
1	AA	966	2MG	C2-N2	5.30	1.45	1.33
22	BA	1962	5MC	C4-N3	5.28	1.43	1.34
1	AA	527	G7M	C2-N3	5.26	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1402	4OC	C2-N3	5.26	1.47	1.36
1	AA	1498	UR3	C6-C5	5.24	1.47	1.35
1	AA	1407	5MC	C4-N3	5.18	1.42	1.34
22	BA	1962	5MC	C2-N3	5.14	1.46	1.36
22	BA	2580	PSU	C2-N3	5.10	1.46	1.37
1	AA	1207	2MG	C2-N2	5.10	1.44	1.33
1	AA	1407	5MC	C2-N3	5.09	1.46	1.36
22	BA	1915	3TD	C1'-C5	-5.08	1.38	1.50
22	BA	2552	OMU	C6-C5	4.94	1.46	1.35
22	BA	2498	OMC	C2-N3	4.90	1.46	1.36
22	BA	2498	OMC	C6-C5	4.83	1.46	1.35
22	BA	1915	3TD	C6-N1	4.78	1.44	1.36
1	AA	527	G7M	C4-N3	4.74	1.48	1.37
1	AA	1207	2MG	C4-N3	4.72	1.48	1.37
22	BA	745	1MG	C4-N3	4.69	1.48	1.37
22	BA	2445	2MG	C5-C4	-4.67	1.31	1.43
1	AA	966	2MG	C2-N1	4.63	1.44	1.36
1	AA	516	PSU	C6-N1	4.59	1.43	1.36
1	AA	1498	UR3	O4-C4	-4.50	1.13	1.23
22	BA	2069	G7M	C2-N3	4.47	1.44	1.33
1	AA	966	2MG	C4-N3	4.46	1.48	1.37
1	AA	1516	2MG	C2-N2	4.45	1.43	1.33
1	AA	1207	2MG	C2-N1	4.40	1.43	1.36
22	BA	1917	PSU	C6-N1	4.39	1.43	1.36
1	AA	967	5MC	C4-N4	4.35	1.45	1.34
22	BA	1911	PSU	C6-N1	4.34	1.43	1.36
22	BA	746	PSU	C6-N1	4.27	1.43	1.36
22	BA	2069	G7M	C4-N3	4.24	1.47	1.37
1	AA	1498	UR3	C2-N3	4.24	1.47	1.39
22	BA	1915	3TD	C2-N3	4.22	1.48	1.38
22	BA	1835	2MG	C2-N2	4.14	1.42	1.33
22	BA	2251	OMG	C4-N3	4.13	1.47	1.37
1	AA	527	G7M	C6-N1	4.06	1.43	1.37
1	AA	1407	5MC	C4-N4	4.05	1.44	1.34
22	BA	2503	2MA	C4-N3	4.05	1.47	1.37
1	AA	967	5MC	C6-N1	3.98	1.44	1.38
1	AA	1516	2MG	C2-N1	3.97	1.43	1.36
22	BA	1835	2MG	C4-N3	3.96	1.47	1.37
22	BA	745	1MG	C2-N2	3.96	1.41	1.34
22	BA	2445	2MG	C2-N2	3.95	1.42	1.33
22	BA	1962	5MC	C4-N4	3.92	1.44	1.34
1	AA	1516	2MG	C4-N3	3.88	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2498	OMC	C4-N4	3.87	1.43	1.33
22	BA	2251	OMG	C2-N2	3.83	1.43	1.34
1	AA	527	G7M	C2-N2	3.81	1.43	1.34
22	BA	955	PSU	C6-N1	3.81	1.42	1.36
1	AA	967	5MC	C2-N1	3.76	1.48	1.40
22	BA	2498	OMC	O2-C2	-3.75	1.16	1.23
1	AA	1516	2MG	C5-C4	-3.74	1.33	1.43
22	BA	1835	2MG	C5-C4	-3.73	1.33	1.43
22	BA	2251	OMG	C5-C4	-3.72	1.33	1.43
22	BA	2580	PSU	C6-N1	3.71	1.42	1.36
22	BA	2251	OMG	C2-N3	3.70	1.42	1.33
22	BA	2552	OMU	O4-C4	-3.69	1.17	1.24
1	AA	1407	5MC	O2-C2	-3.69	1.16	1.23
22	BA	745	1MG	C5-C4	-3.68	1.33	1.43
22	BA	2504	PSU	C6-N1	3.68	1.42	1.36
22	BA	2605	PSU	C6-N1	3.68	1.42	1.36
1	AA	1402	4OC	C4-N4	3.65	1.43	1.35
22	BA	2498	OMC	C4-N3	3.62	1.41	1.34
22	BA	2498	OMC	C2-N1	3.56	1.47	1.40
1	AA	1407	5MC	C6-N1	3.52	1.44	1.38
22	BA	2445	2MG	C4-N3	3.49	1.45	1.37
1	AA	1519	MA6	C5-C4	-3.49	1.31	1.40
1	AA	1402	4OC	C2-N1	3.47	1.47	1.40
1	AA	1518	MA6	C5-C4	-3.43	1.31	1.40
22	BA	746	PSU	O4-C4	-3.43	1.17	1.23
22	BA	2552	OMU	O2-C2	-3.39	1.16	1.23
22	BA	2445	2MG	O6-C6	-3.37	1.16	1.23
22	BA	1962	5MC	O2-C2	-3.35	1.17	1.23
22	BA	2069	G7M	C2-N2	3.34	1.42	1.34
22	BA	1835	2MG	O6-C6	-3.32	1.16	1.23
22	BA	2503	2MA	C5-C4	-3.32	1.34	1.43
22	BA	2030	6MZ	C5-C4	-3.32	1.32	1.40
1	AA	1402	4OC	C5-C4	3.31	1.47	1.40
1	AA	516	PSU	C4-N3	3.27	1.44	1.38
1	AA	1207	2MG	C6-N1	3.25	1.42	1.37
22	BA	1618	6MZ	C5-C4	-3.23	1.32	1.40
22	BA	2251	OMG	O6-C6	-3.20	1.16	1.23
34	BM	81	4D4	CZ-NH2	3.19	1.45	1.32
1	AA	1498	UR3	O2-C2	-3.19	1.16	1.22
22	BA	2604	PSU	C6-N1	3.17	1.41	1.36
22	BA	955	PSU	O4-C4	-3.15	1.17	1.23
22	BA	1835	2MG	C2-N1	3.14	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C5-C6	3.14	1.53	1.45
22	BA	745	1MG	O6-C6	-3.12	1.16	1.22
1	AA	966	2MG	C5-C4	-3.11	1.35	1.43
22	BA	746	PSU	C4-N3	3.11	1.44	1.38
22	BA	2580	PSU	O4-C4	-3.10	1.17	1.23
1	AA	1402	4OC	O2-C2	-3.09	1.18	1.23
22	BA	2069	G7M	C6-N1	3.08	1.42	1.37
1	AA	967	5MC	O2-C2	-3.04	1.18	1.23
22	BA	2457	PSU	C6-N1	3.01	1.41	1.36
1	AA	966	2MG	C6-N1	3.01	1.42	1.37
1	AA	1407	5MC	C2-N1	3.00	1.46	1.40
22	BA	2580	PSU	O4'-C1'	-2.98	1.39	1.43
1	AA	1207	2MG	C5-C4	-2.96	1.35	1.43
22	BA	2604	PSU	O4-C4	-2.93	1.18	1.23
22	BA	1917	PSU	C4-N3	2.92	1.44	1.38
1	AA	1498	UR3	C5-C4	2.90	1.51	1.43
22	BA	1962	5MC	C2-N1	2.85	1.46	1.40
22	BA	2605	PSU	O4-C4	-2.84	1.18	1.23
1	AA	1516	2MG	O6-C6	-2.84	1.17	1.23
22	BA	1911	PSU	C4-N3	2.84	1.44	1.38
1	AA	1402	4OC	C6-N1	2.82	1.44	1.38
22	BA	1911	PSU	O4-C4	-2.82	1.18	1.23
22	BA	2457	PSU	O4-C4	-2.82	1.18	1.23
1	AA	1516	2MG	C6-N1	2.82	1.42	1.37
22	BA	1962	5MC	C6-N1	2.80	1.42	1.38
22	BA	2504	PSU	O4-C4	-2.79	1.18	1.23
22	BA	2504	PSU	C4-N3	2.69	1.43	1.38
22	BA	1939	5MU	C4-C5	-2.64	1.40	1.44
1	AA	516	PSU	O4'-C1'	-2.61	1.40	1.43
1	AA	1498	UR3	C3U-N3	-2.60	1.42	1.47
25	BD	150	MEQ	OE1-CD	-2.60	1.18	1.23
22	BA	2445	2MG	C2-N1	2.60	1.40	1.36
22	BA	1917	PSU	O4-C4	-2.58	1.18	1.23
22	BA	2030	6MZ	C4-N3	-2.56	1.32	1.35
34	BM	81	4D4	CZ-NH1	-2.56	1.24	1.34
22	BA	1618	6MZ	C2-N3	2.55	1.36	1.32
1	AA	1207	2MG	O6-C6	-2.54	1.18	1.23
22	BA	1915	3TD	O2-C2	-2.52	1.18	1.23
22	BA	955	PSU	C4-N3	2.52	1.43	1.38
22	BA	1618	6MZ	C4-N3	-2.52	1.32	1.35
22	BA	2069	G7M	C5-C4	-2.49	1.34	1.39
22	BA	2030	6MZ	C6-N1	-2.47	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C2-N1	2.46	1.43	1.37
1	AA	966	2MG	O6-C6	-2.45	1.18	1.23
1	AA	1207	2MG	C5-C6	2.44	1.52	1.47
22	BA	2605	PSU	C4-N3	2.43	1.43	1.38
22	BA	2457	PSU	O4'-C1'	-2.41	1.40	1.43
22	BA	2498	OMC	C6-N1	2.39	1.43	1.38
1	AA	516	PSU	O4-C4	-2.38	1.19	1.23
22	BA	2552	OMU	C4-N3	2.38	1.42	1.38
22	BA	2503	2MA	C2-N1	2.35	1.43	1.36
1	AA	1518	MA6	C6-N1	-2.34	1.29	1.33
1	AA	1519	MA6	C6-N1	-2.29	1.29	1.33
22	BA	1618	6MZ	C9-N6	2.28	1.49	1.45
22	BA	1915	3TD	O4-C4	-2.28	1.18	1.23
25	BD	150	MEQ	CD-NE2	2.23	1.44	1.34
22	BA	1939	5MU	C5M-C5	-2.22	1.45	1.50
1	AA	1518	MA6	C4-N3	-2.21	1.32	1.35
22	BA	746	PSU	C1'-C5	2.20	1.55	1.50
34	BM	81	4D4	OB-CB	-2.20	1.38	1.43
22	BA	2604	PSU	C4-N3	2.15	1.42	1.38
1	AA	966	2MG	C5-C6	2.15	1.51	1.47
22	BA	2030	6MZ	C5-N7	-2.14	1.32	1.39
1	AA	1498	UR3	C6-N1	2.14	1.43	1.38
22	BA	1911	PSU	O4'-C1'	-2.14	1.40	1.43
1	AA	1518	MA6	C10-N6	-2.14	1.40	1.45
22	BA	2030	6MZ	C9-N6	2.12	1.48	1.45
22	BA	2605	PSU	O2-C2	-2.11	1.19	1.23
22	BA	2503	2MA	C6-N1	2.11	1.42	1.38
22	BA	1939	5MU	C4-N3	-2.11	1.34	1.38
22	BA	2552	OMU	C6-N1	2.10	1.43	1.38
1	AA	1519	MA6	C4-N3	-2.10	1.32	1.35
22	BA	2457	PSU	C4-N3	2.08	1.42	1.38
1	AA	1518	MA6	C5-N7	-2.08	1.32	1.39
22	BA	2580	PSU	C4-N3	2.06	1.42	1.38
22	BA	2605	PSU	O4'-C1'	-2.04	1.41	1.43
22	BA	746	PSU	O4'-C1'	-2.04	1.41	1.43

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-14.58	101.71	117.06
1	AA	1518	MA6	N1-C6-N6	-13.26	103.10	117.06
22	BA	2030	6MZ	C9-N6-C6	-8.27	115.75	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1618	6MZ	C9-N6-C6	-7.09	116.76	122.87
22	BA	1618	6MZ	N3-C2-N1	-6.64	118.29	128.68
22	BA	2604	PSU	N1-C2-N3	6.40	122.38	115.13
22	BA	2604	PSU	C6-C5-C4	6.25	122.57	118.20
22	BA	2552	OMU	C4-N3-C2	-6.17	118.45	126.58
22	BA	2457	PSU	N1-C2-N3	6.12	122.06	115.13
1	AA	1519	MA6	N3-C2-N1	-6.06	119.20	128.68
22	BA	2604	PSU	C4-N3-C2	-5.82	117.95	126.34
22	BA	2457	PSU	C4-N3-C2	-5.79	118.00	126.34
1	AA	1498	UR3	C4-N3-C2	-5.65	119.24	124.56
1	AA	1518	MA6	N3-C2-N1	-5.62	119.89	128.68
22	BA	2445	2MG	CM2-N2-C2	-5.61	111.46	123.86
22	BA	2030	6MZ	N3-C2-N1	-5.60	119.92	128.68
22	BA	955	PSU	N1-C2-N3	5.58	121.45	115.13
22	BA	1915	3TD	N1-C2-N3	5.46	120.45	116.14
22	BA	1911	PSU	C4-N3-C2	-5.44	118.51	126.34
22	BA	2605	PSU	C4-N3-C2	-5.32	118.68	126.34
22	BA	955	PSU	C4-N3-C2	-5.28	118.73	126.34
22	BA	1911	PSU	N1-C2-N3	5.11	120.92	115.13
22	BA	746	PSU	C4-N3-C2	-5.11	118.97	126.34
22	BA	2552	OMU	N3-C2-N1	5.11	121.67	114.89
22	BA	1618	6MZ	C2-N1-C6	5.05	120.92	116.59
12	AL	89	D2T	CB1-SB-CB	4.91	111.32	102.44
22	BA	2580	PSU	N1-C2-N3	4.74	120.50	115.13
22	BA	1917	PSU	N1-C2-N3	4.65	120.40	115.13
22	BA	2604	PSU	O2-C2-N1	-4.65	117.67	122.79
1	AA	516	PSU	C4-N3-C2	-4.61	119.69	126.34
22	BA	2445	2MG	C5-C6-N1	4.55	121.99	113.95
22	BA	1917	PSU	C4-N3-C2	-4.53	119.81	126.34
22	BA	2605	PSU	N1-C2-N3	4.53	120.26	115.13
22	BA	2030	6MZ	C2-N1-C6	4.51	120.46	116.59
22	BA	2504	PSU	C4-N3-C2	-4.50	119.86	126.34
1	AA	1407	5MC	C5-C6-N1	-4.45	118.76	123.34
22	BA	745	1MG	C5-C6-N1	4.44	120.58	113.90
22	BA	2580	PSU	C4-N3-C2	-4.33	120.11	126.34
22	BA	2457	PSU	C6-C5-C4	4.27	121.19	118.20
22	BA	1915	3TD	C4-N3-C2	-4.24	120.00	124.61
1	AA	516	PSU	N1-C2-N3	4.20	119.88	115.13
22	BA	1911	PSU	C6-C5-C4	4.17	121.11	118.20
22	BA	1835	2MG	C5-C6-N1	4.16	121.30	113.95
22	BA	1835	2MG	CM2-N2-C2	-4.14	114.71	123.86
22	BA	955	PSU	C6-N1-C2	-4.10	118.49	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	516	PSU	C6-C5-C4	4.04	121.03	118.20
22	BA	955	PSU	C6-C5-C4	4.01	121.00	118.20
22	BA	2504	PSU	N1-C2-N3	3.96	119.61	115.13
22	BA	2580	PSU	C6-N1-C2	-3.91	118.68	122.68
1	AA	1516	2MG	C5-C6-N1	3.90	120.83	113.95
1	AA	1516	2MG	CM2-N2-C2	-3.83	115.41	123.86
22	BA	2605	PSU	C6-C5-C4	3.78	120.84	118.20
22	BA	1917	PSU	C6-N1-C2	-3.77	118.82	122.68
22	BA	1618	6MZ	C1'-N9-C4	-3.72	120.11	126.64
22	BA	2457	PSU	O2-C2-N1	-3.70	118.72	122.79
1	AA	1207	2MG	C5-C6-N1	3.69	120.46	113.95
22	BA	2604	PSU	C6-N1-C2	-3.68	118.92	122.68
22	BA	746	PSU	N1-C2-N3	3.58	119.19	115.13
22	BA	2552	OMU	C5-C4-N3	3.55	120.15	114.84
22	BA	2457	PSU	C6-N1-C2	-3.53	119.08	122.68
1	AA	1516	2MG	O6-C6-C5	-3.43	117.67	124.37
22	BA	2251	OMG	C5-C6-N1	3.42	119.99	113.95
22	BA	2503	2MA	C5-C6-N1	3.41	119.90	114.02
1	AA	967	5MC	C5-C6-N1	-3.31	119.94	123.34
1	AA	527	G7M	C2-N1-C6	-3.28	119.06	125.10
22	BA	2030	6MZ	C1'-N9-C4	-3.27	120.90	126.64
1	AA	966	2MG	C5-C6-N1	3.20	119.61	113.95
22	BA	1917	PSU	C6-C5-C4	3.17	120.42	118.20
12	AL	89	D2T	OD2-CG-CB	3.15	119.96	113.15
22	BA	1939	5MU	C4-N3-C2	-3.10	123.34	127.35
22	BA	1911	PSU	C6-N1-C2	-3.08	119.53	122.68
22	BA	747	5MU	C4-N3-C2	-3.05	123.41	127.35
22	BA	1939	5MU	C6-C5-C4	3.00	120.54	118.03
22	BA	2503	2MA	N1-C2-N3	-2.98	118.11	123.06
22	BA	1962	5MC	C5-C6-N1	-2.95	120.30	123.34
22	BA	1962	5MC	CM5-C5-C6	-2.90	118.97	122.85
22	BA	2503	2MA	CM2-C2-N1	2.89	122.66	116.23
1	AA	516	PSU	C6-N1-C2	-2.88	119.74	122.68
22	BA	2503	2MA	C8-N7-C5	2.87	108.45	102.99
22	BA	1939	5MU	C5-C4-N3	2.83	117.73	115.31
22	BA	2069	G7M	C2-N1-C6	-2.83	119.89	125.10
22	BA	2504	PSU	C6-C5-C4	2.77	120.13	118.20
22	BA	2580	PSU	C6-C5-C4	2.75	120.12	118.20
22	BA	745	1MG	C8-N7-C5	2.69	108.11	102.99
1	AA	966	2MG	C8-N7-C5	2.67	108.08	102.99
22	BA	2251	OMG	C2-N1-C6	-2.66	120.20	125.10
22	BA	1835	2MG	O6-C6-C5	-2.64	119.22	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2445	2MG	O6-C6-C5	-2.63	119.23	124.37
22	BA	955	PSU	O2-C2-N1	-2.62	119.91	122.79
22	BA	2552	OMU	O2-C2-N1	-2.61	119.31	122.79
1	AA	1516	2MG	C8-N7-C5	2.58	107.90	102.99
22	BA	2251	OMG	C8-N7-C5	2.58	107.90	102.99
22	BA	746	PSU	O2-C2-N1	-2.56	119.97	122.79
22	BA	2445	2MG	C8-N7-C5	2.56	107.87	102.99
1	AA	1207	2MG	C8-N7-C5	2.55	107.84	102.99
22	BA	747	5MU	C6-C5-C4	2.44	120.07	118.03
22	BA	2504	PSU	C6-N1-C2	-2.42	120.21	122.68
25	BD	150	MEQ	CG-CD-NE2	2.42	119.64	116.29
1	AA	1207	2MG	O6-C6-C5	-2.40	119.68	124.37
22	BA	2552	OMU	O4-C4-C5	-2.39	120.95	125.16
1	AA	516	PSU	O4'-C1'-C2'	2.39	108.51	105.14
1	AA	516	PSU	O2-C2-N1	-2.39	120.16	122.79
22	BA	2069	G7M	N2-C2-N1	2.35	121.72	116.71
22	BA	1939	5MU	C5-C6-N1	-2.33	120.94	123.34
1	AA	966	2MG	CM2-N2-C2	-2.33	118.73	123.86
22	BA	746	PSU	C5-C4-N3	2.31	121.81	116.58
22	BA	2552	OMU	C2'-C1'-N1	-2.30	109.77	114.22
1	AA	966	2MG	O6-C6-C5	-2.27	119.93	124.37
22	BA	2498	OMC	O2-C2-N3	-2.27	118.64	122.33
22	BA	1835	2MG	C8-N7-C5	2.26	107.30	102.99
22	BA	746	PSU	C6-N1-C2	-2.26	120.37	122.68
1	AA	1407	5MC	CM5-C5-C6	-2.25	119.84	122.85
34	BM	81	4D4	CB-CA-C	-2.23	108.21	111.77
1	AA	1402	4OC	CM4-N4-C4	-2.21	118.12	122.45
22	BA	2251	OMG	O6-C6-C5	-2.21	120.06	124.37
22	BA	1917	PSU	O2-C2-N1	-2.19	120.38	122.79
1	AA	1498	UR3	C3U-N3-C2	2.16	121.10	117.31
22	BA	745	1MG	C2-N1-C6	-2.14	119.21	120.95
22	BA	2605	PSU	C6-N1-C2	-2.10	120.53	122.68
22	BA	1915	3TD	C6-C5-C4	2.10	119.67	118.22
1	AA	1402	4OC	C6-C5-C4	2.09	119.52	116.96
22	BA	2251	OMG	N2-C2-N1	2.07	121.11	116.71
22	BA	746	PSU	O4-C4-C5	-2.05	118.68	124.05
12	AL	89	D2T	OD2-CG-OD1	-2.05	119.44	124.09
22	BA	2604	PSU	C5-C6-N1	-2.03	119.07	122.11
22	BA	2498	OMC	C6-C5-C4	2.01	120.74	117.50
22	BA	1911	PSU	O4'-C1'-C2'	2.00	107.97	105.14

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
25	BD	150	MEQ	O-C-CA-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	747	5MU	C3'-C4'-C5'-O5'
22	BA	1915	3TD	C3'-C4'-C5'-O5'
22	BA	1915	3TD	O4'-C4'-C5'-O5'
22	BA	2251	OMG	C1'-C2'-O2'-CM2
22	BA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
22	BA	747	5MU	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
22	BA	2580	PSU	O4'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2580	PSU	C3'-C4'-C5'-O5'
25	BD	150	MEQ	OE1-CD-CG-CB
25	BD	150	MEQ	NE2-CD-CG-CB
22	BA	2445	2MG	O4'-C4'-C5'-O5'
22	BA	2503	2MA	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
22	BA	2069	G7M	C4'-C5'-O5'-P
25	BD	150	MEQ	N-CA-CB-CG
22	BA	747	5MU	C4'-C5'-O5'-P
34	BM	81	4D4	OB-CB-CG-CD
22	BA	746	PSU	O4'-C4'-C5'-O5'
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	746	PSU	O4'-C1'-C5-C6
1	AA	516	PSU	O4'-C4'-C5'-O5'
22	BA	1917	PSU	O4'-C4'-C5'-O5'
22	BA	2503	2MA	C3'-C4'-C5'-O5'
34	BM	81	4D4	O-C-CA-CB
22	BA	2251	OMG	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BA	2251	OMG	1	0
22	BA	2030	6MZ	2	0
1	AA	1207	2MG	1	0
1	AA	1516	2MG	1	0
22	BA	2498	OMC	1	0
34	BM	81	4D4	1	0
25	BD	150	MEQ	1	0
1	AA	1519	MA6	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 490 ligands modelled in this entry, 489 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	TRP	BA	3001	-	14,16,16	0.84	1 (7%)	16,22,22	1.04	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TRP	BA	3001	-	-	0/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3001	TRP	OXT-C	-2.11	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BA	3001	TRP	OXT-C-O	-2.32	118.81	124.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2
54	B7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.97
1	BA	2099:U	O3'	2100:G	P	3.25
1	B7	7:U	O3'	8:G	P	2.92

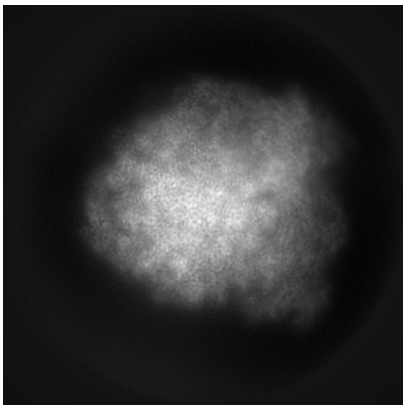
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12695. These allow visual inspection of the internal detail of the map and identification of artifacts.

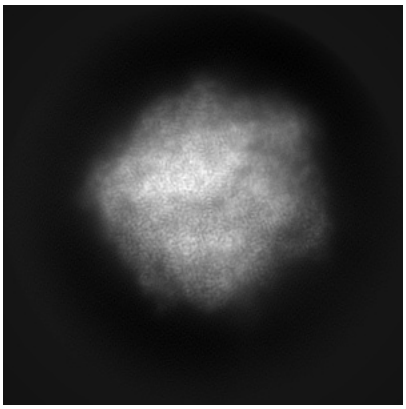
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

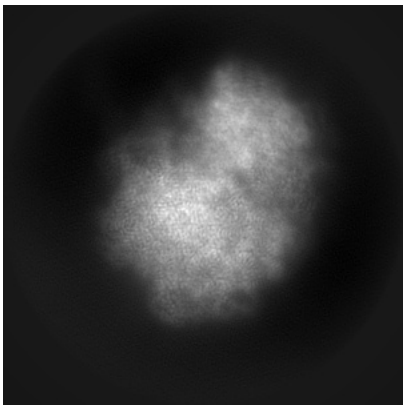
6.1.1 Primary map



X

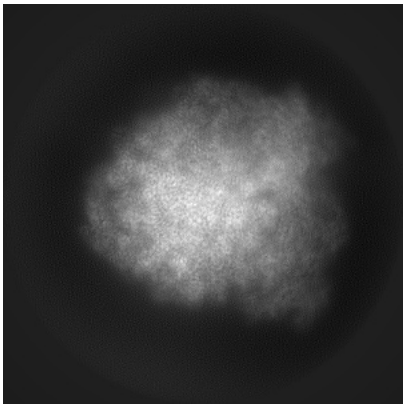


Y

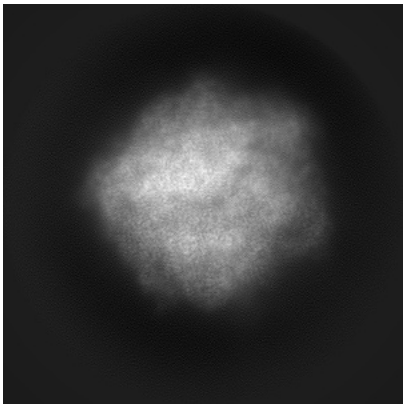


Z

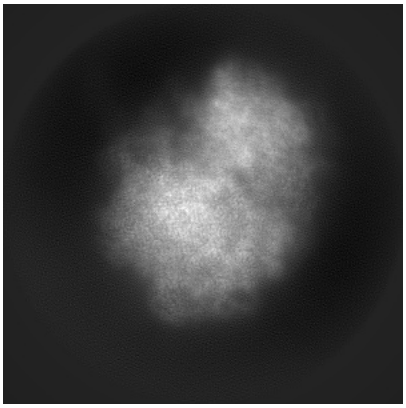
6.1.2 Raw map



X



Y

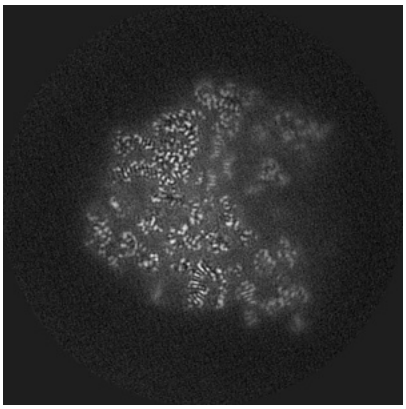


Z

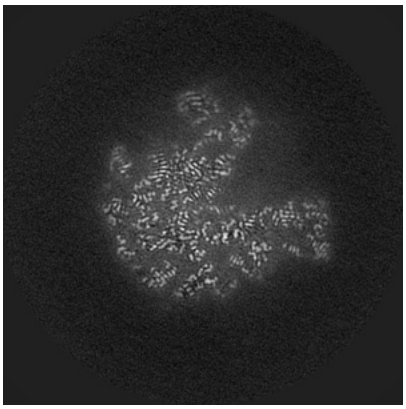
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

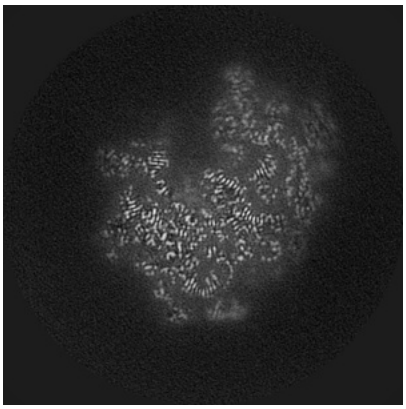
6.2.1 Primary map



X Index: 204

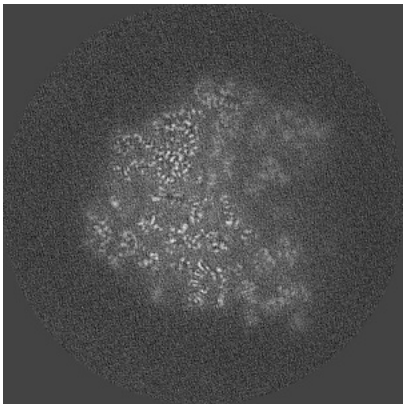


Y Index: 204

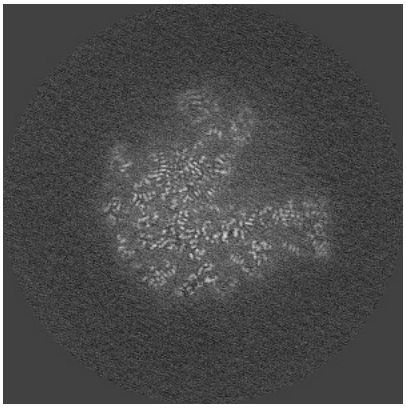


Z Index: 204

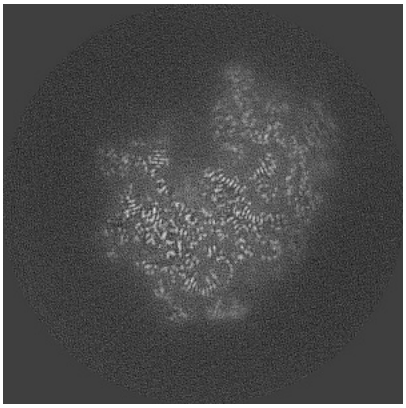
6.2.2 Raw map



X Index: 204



Y Index: 204

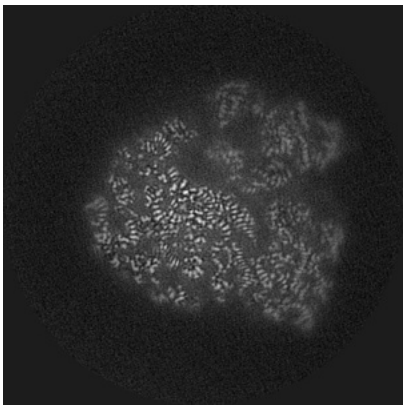


Z Index: 204

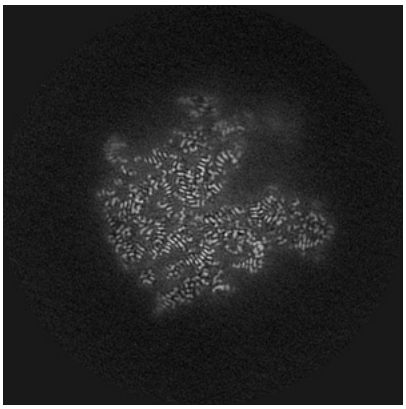
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

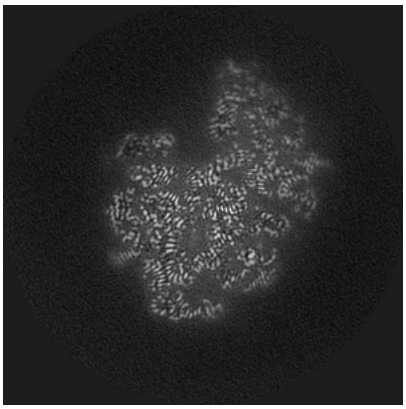
6.3.1 Primary map



X Index: 219

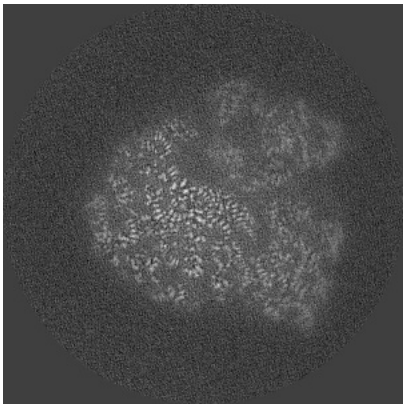


Y Index: 195

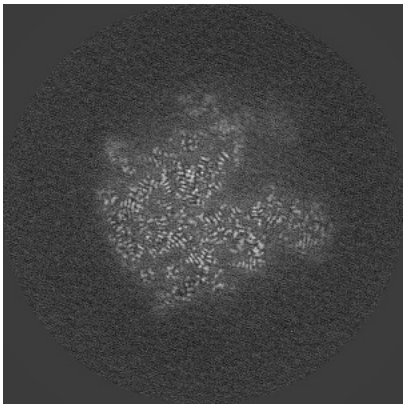


Z Index: 188

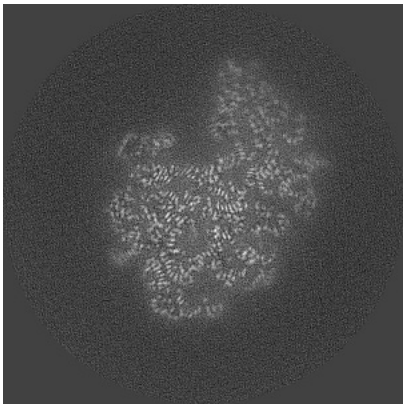
6.3.2 Raw map



X Index: 219



Y Index: 196

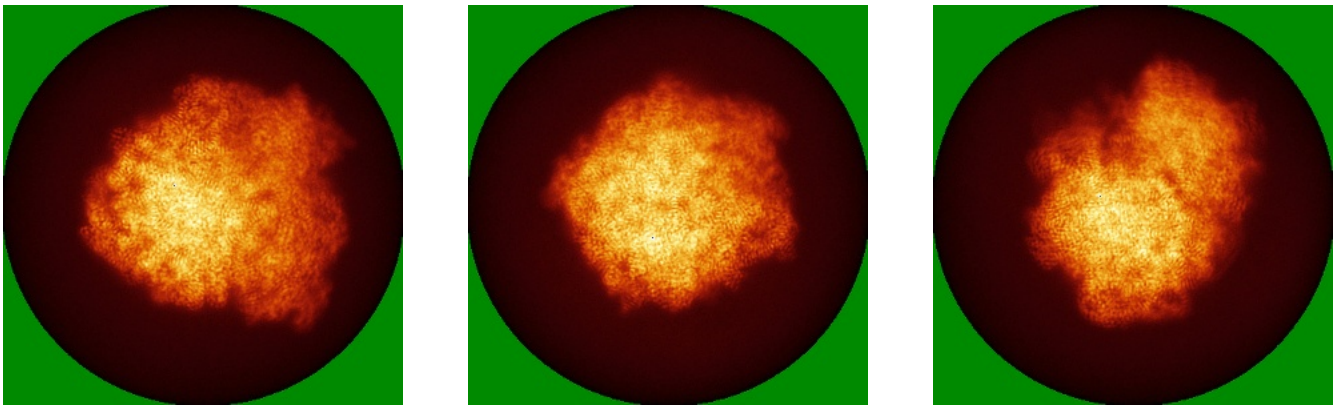


Z Index: 187

The images above show the largest variance slices of the map in three orthogonal directions.

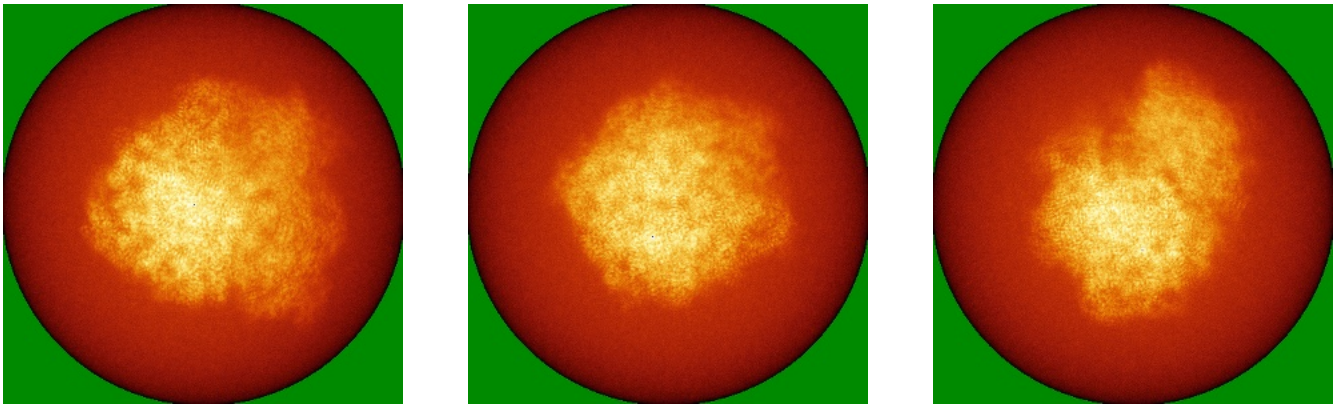
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

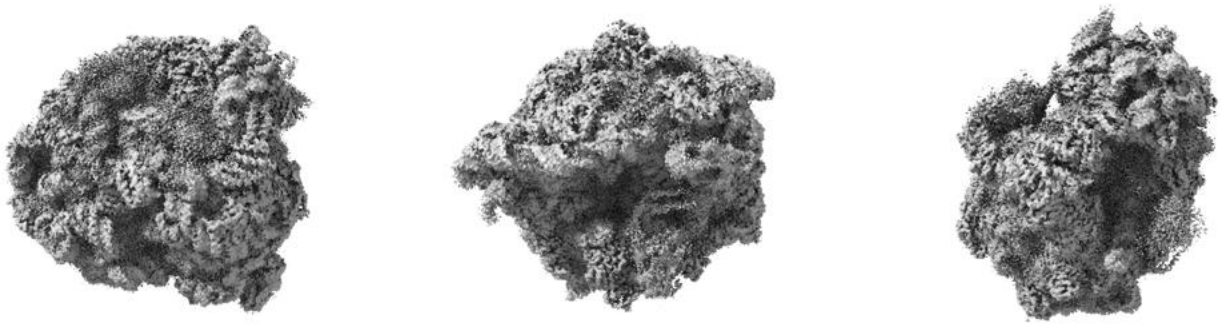


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

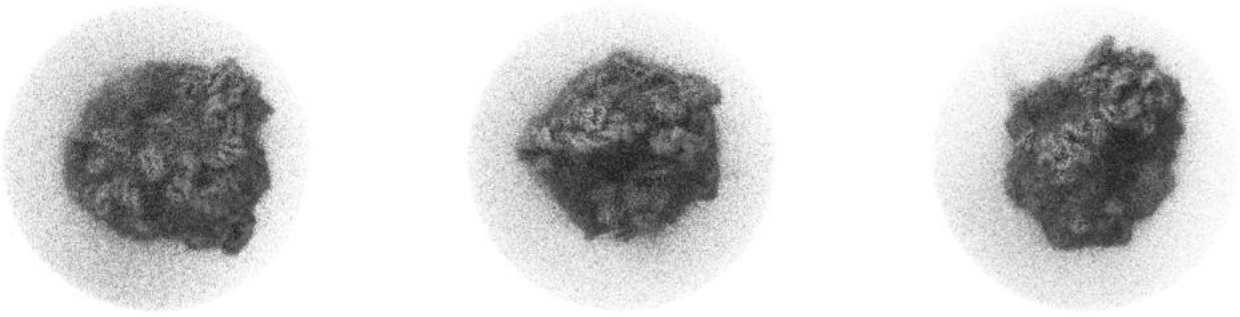
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

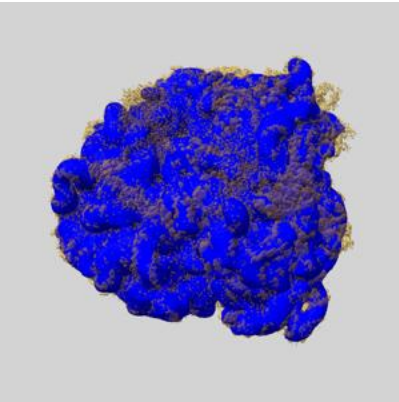
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

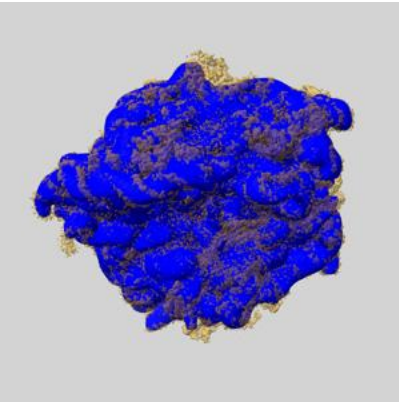
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

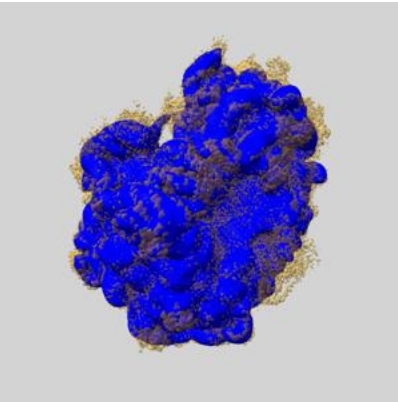
6.6.1 emd_12695_msk_1.map



X



Y

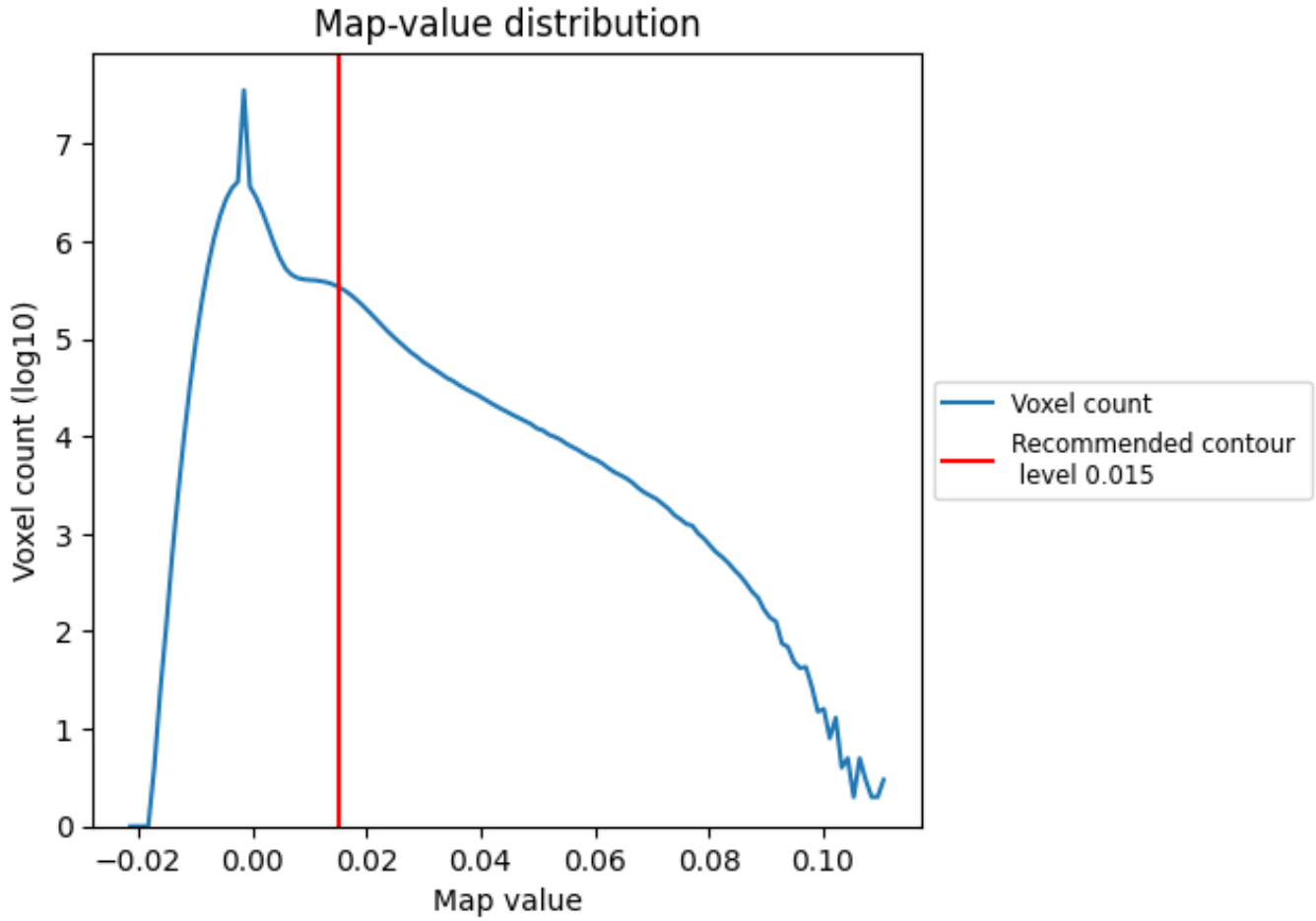


Z

7 Map analysis

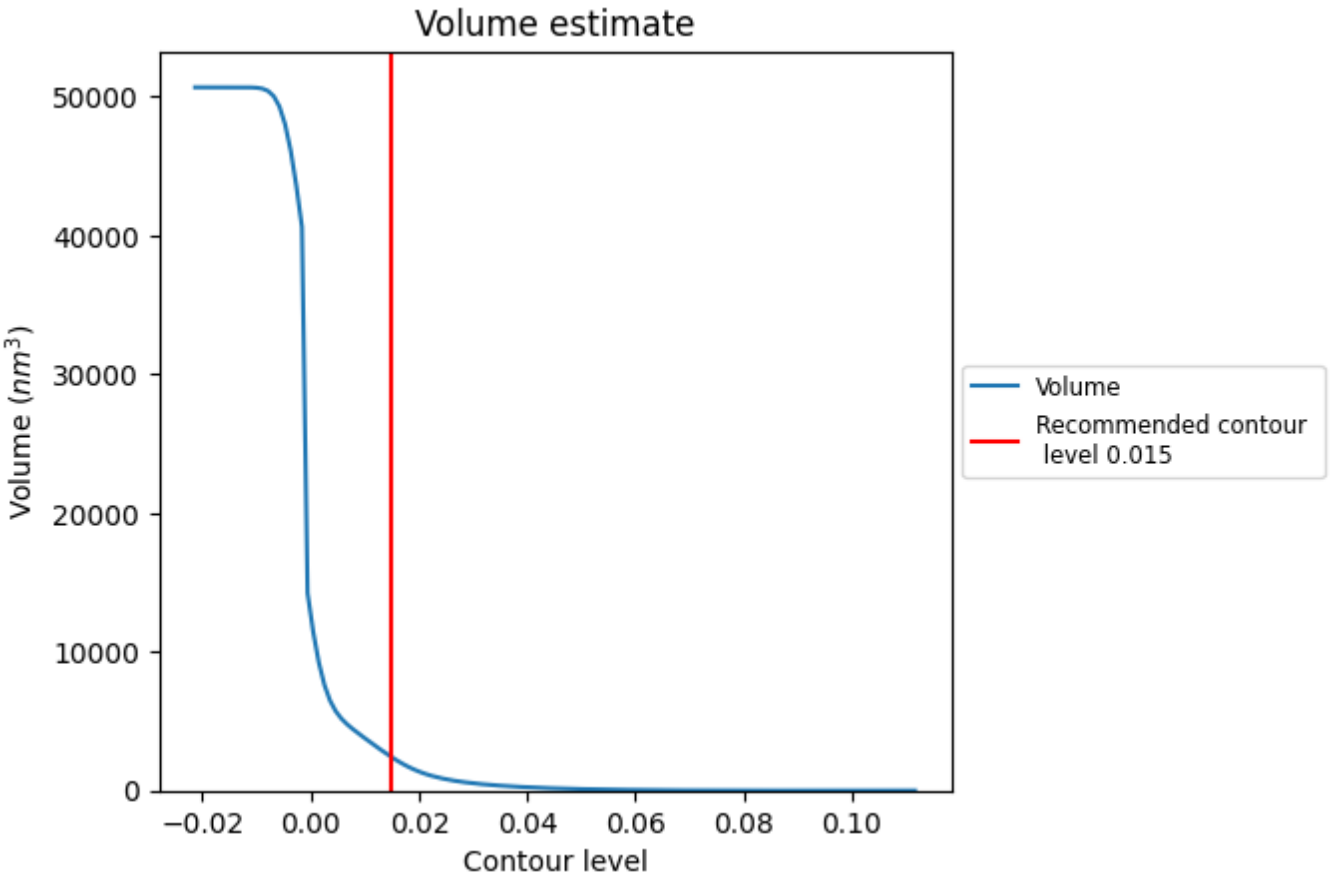
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

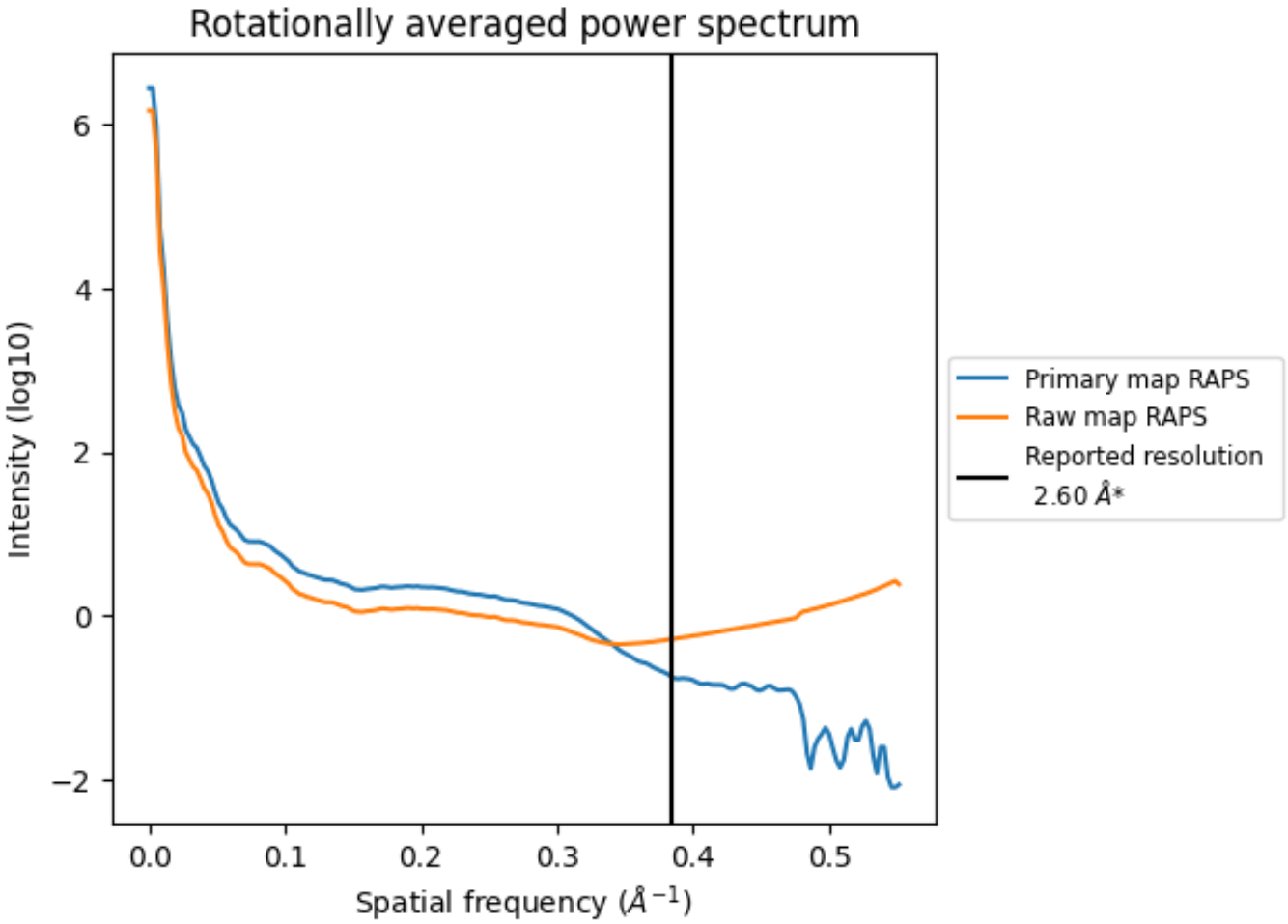
7.2 Volume estimate



The volume at the recommended contour level is 2396 nm^3; this corresponds to an approximate mass of 2165 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

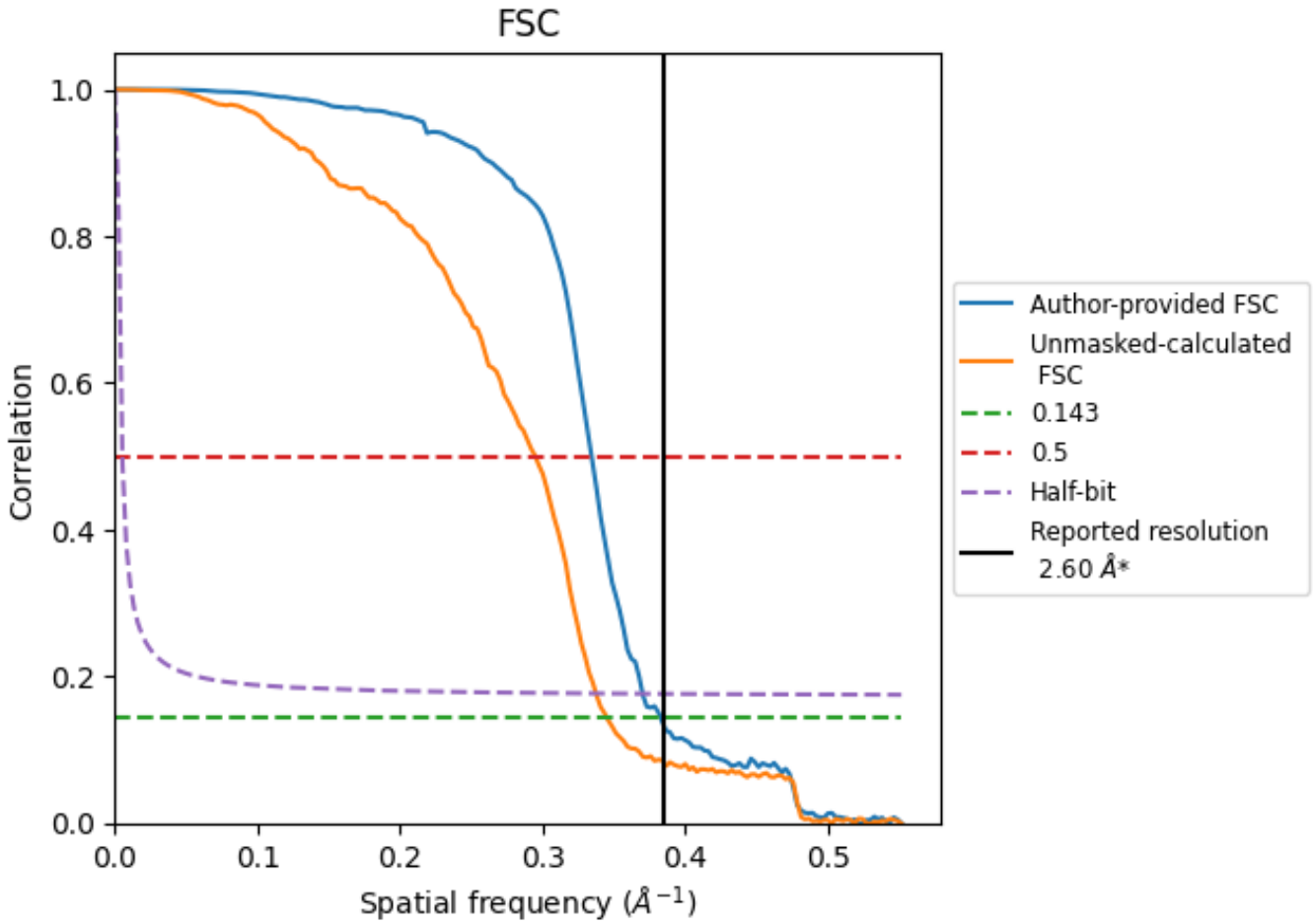


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

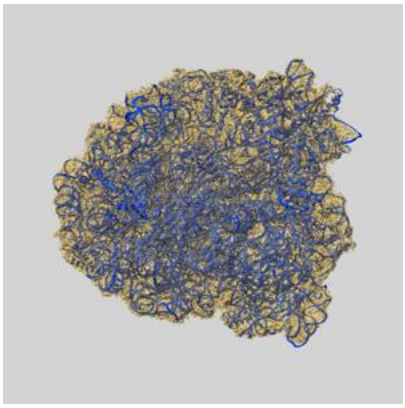
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.99	2.70
Unmasked-calculated*	2.90	3.39	2.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.90 differs from the reported value 2.6 by more than 10 %

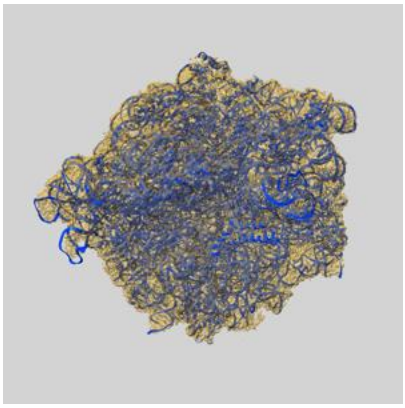
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12695 and PDB model 7O1C. Per-residue inclusion information can be found in section 3 on page 16.

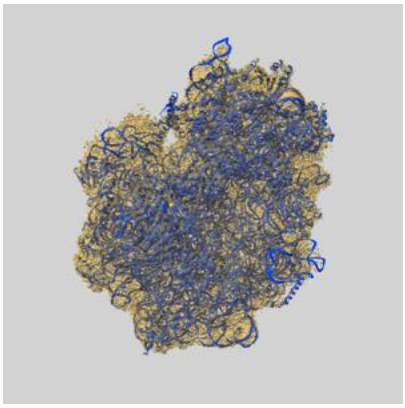
9.1 Map-model overlay



X



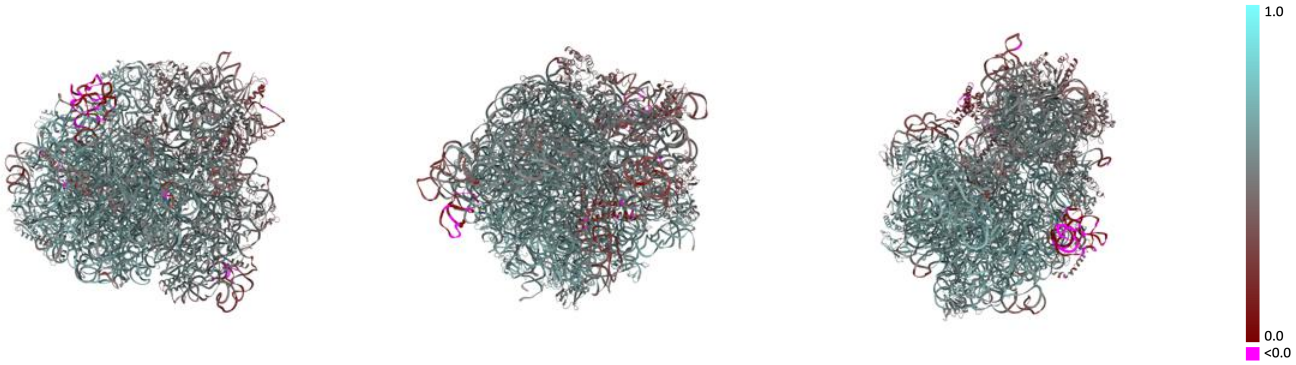
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

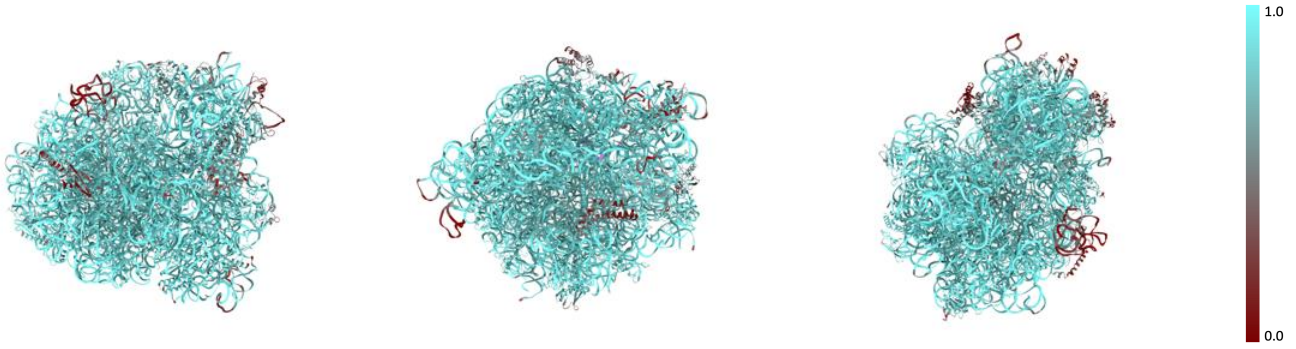
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

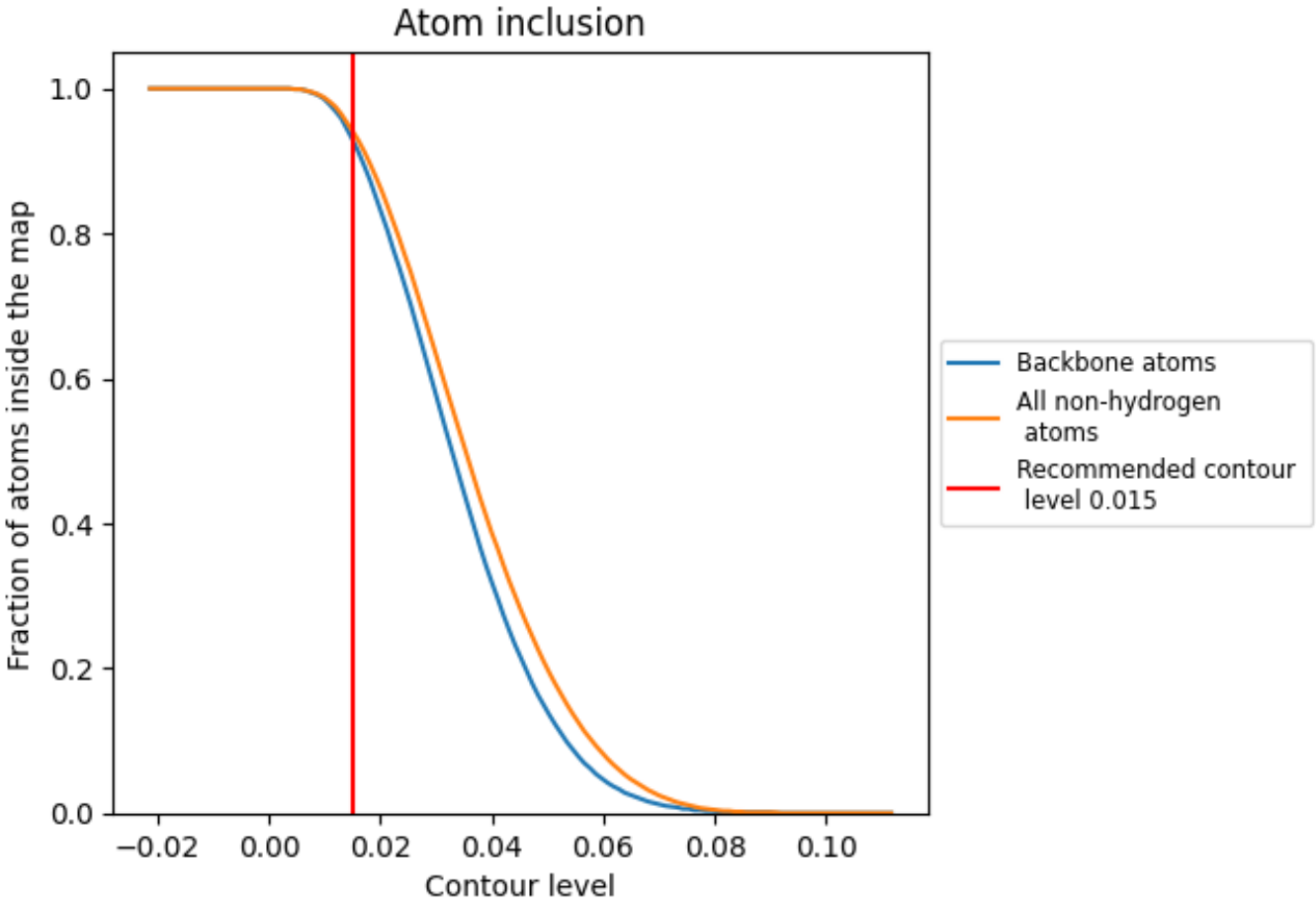
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.5550
AA	0.9590	0.5270
AB	0.5960	0.3870
AC	0.8500	0.4360
AD	0.8410	0.4500
AE	0.9450	0.5100
AF	0.8810	0.4910
AG	0.8140	0.4290
AH	0.9090	0.5090
AI	0.7840	0.4280
AJ	0.6360	0.3580
AK	0.9530	0.5230
AL	0.9760	0.5520
AM	0.8510	0.4580
AN	0.9040	0.4500
AO	0.9360	0.5230
AP	0.9120	0.4960
AQ	0.9450	0.5040
AR	0.9540	0.5240
AS	0.8330	0.4340
AT	0.9340	0.5270
AU	0.8760	0.4540
B0	0.9740	0.6090
B1	0.9800	0.5780
B2	1.0000	0.6340
B3	1.0000	0.6300
B4	0.9930	0.6200
B5	1.0000	0.5670
B7	1.0000	0.5200
B8	0.9990	0.4730
B9	0.7580	0.3640
BA	0.9710	0.5970
BB	0.9840	0.5930
BC	0.9970	0.6310
BD	0.9730	0.6200

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BE	0.8800	0.5710
BF	0.9070	0.4950
BG	0.8610	0.5360
BH	0.4520	0.3840
BI	0.5510	0.3810
BJ	0.9810	0.6150
BK	0.9910	0.6060
BL	0.9570	0.5940
BM	0.9950	0.6130
BN	0.9910	0.6310
BO	0.9280	0.5730
BP	0.9720	0.6060
BQ	0.9880	0.6250
BR	0.9250	0.5830
BS	0.9800	0.6040
BT	0.9650	0.5770
BU	0.9200	0.5460
BV	0.9210	0.5930
BW	0.9810	0.6060
BX	0.9870	0.6060
BY	0.9180	0.5440
BZ	0.9430	0.5870